

# **Novel exocyclic enamides: synthesis and evaluation of fungicidal activities of 5-methylene-2-(trifluoromethyl)morpholin-3-one derivatives**

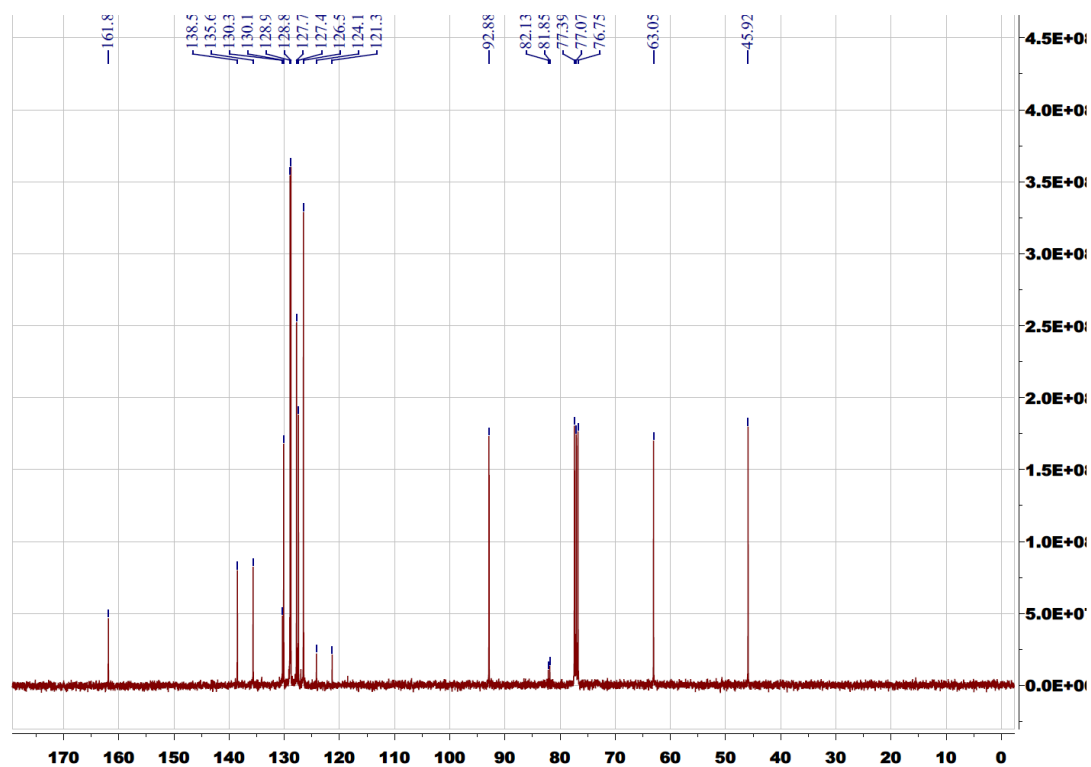
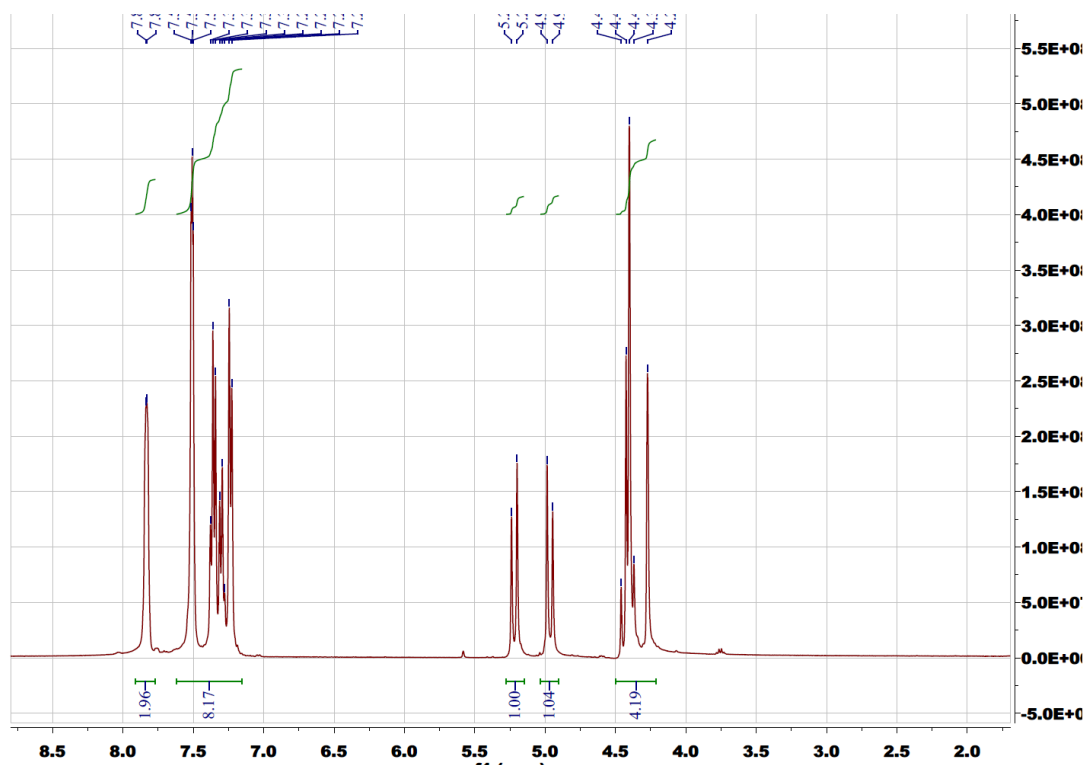
**Can Cui, Cong Zhu, Lei Tian, Hui-Hui Yang, Jian-Qiang, Wei-Guang Zhao\***

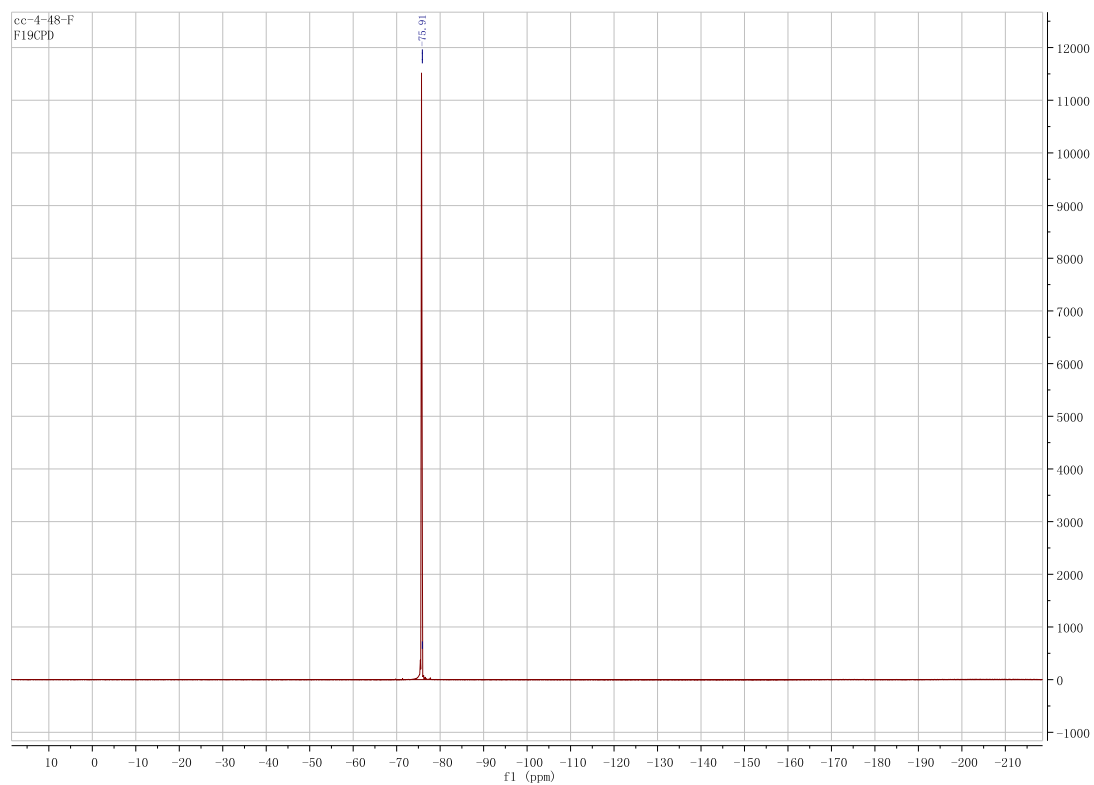
State Key Laboratory of Elemento-Organic Chemistry, Collaborative Innovation Center of Chemical Science and Engineering, Nankai University, Tianjin 300071, China. E-mail: [zwg@nankai.edu.cn](mailto:zwg@nankai.edu.cn).

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2a

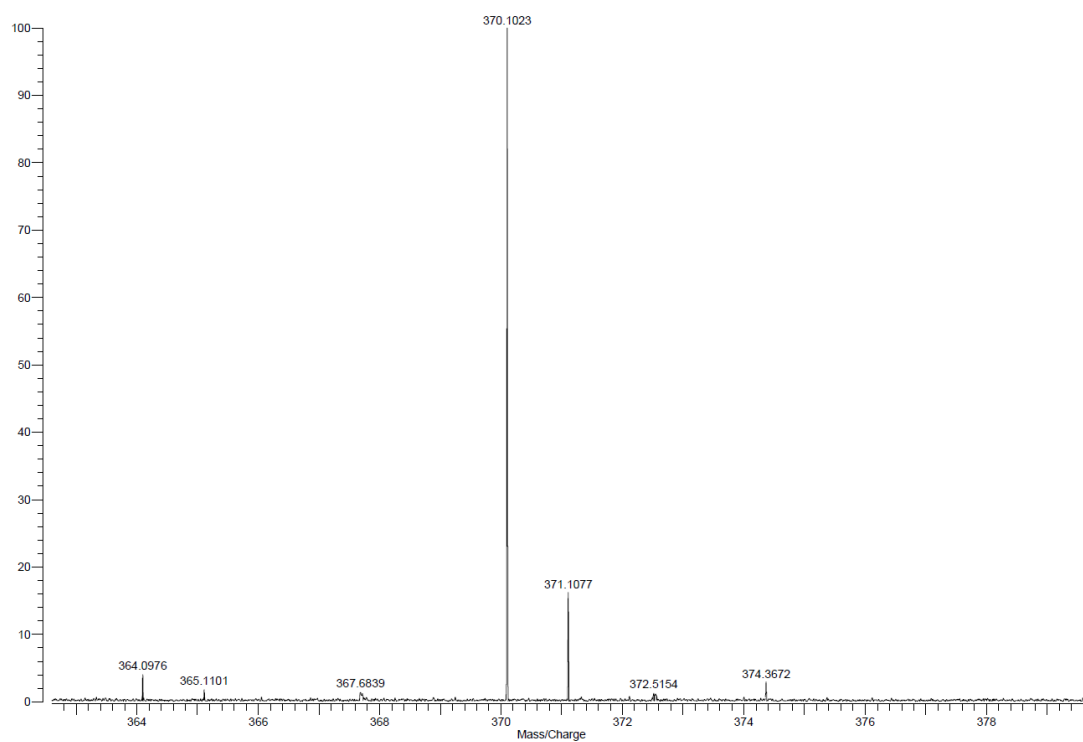




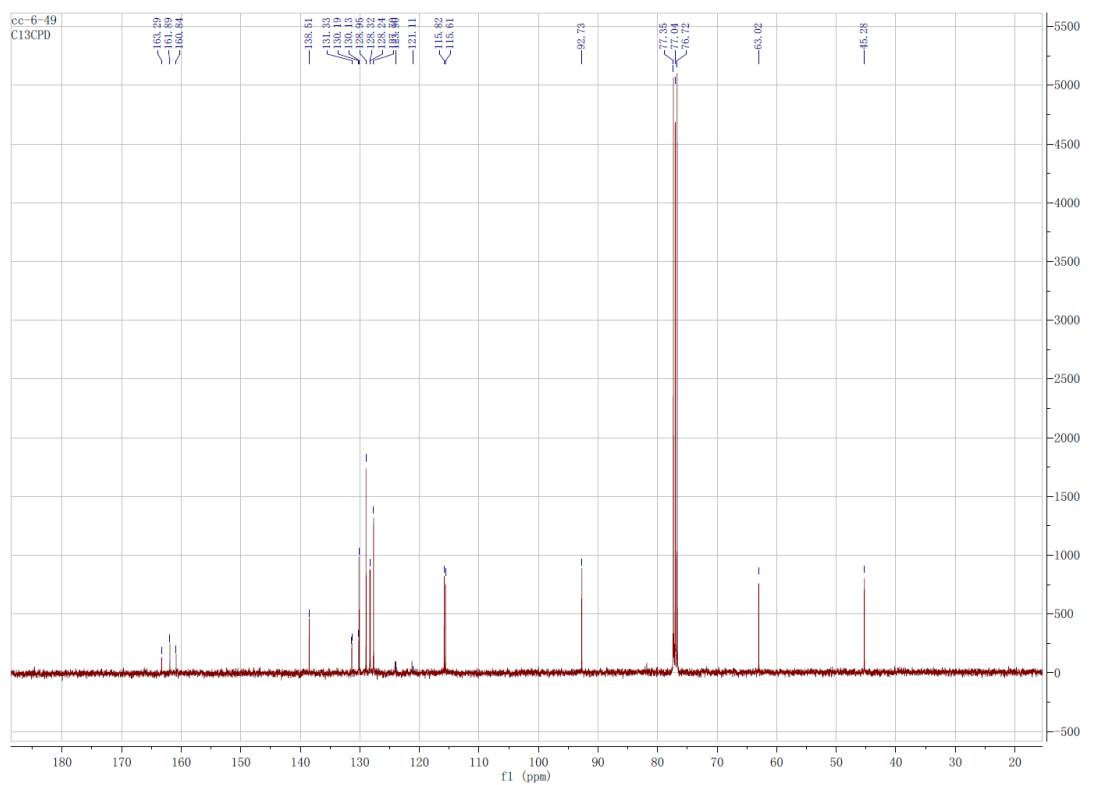
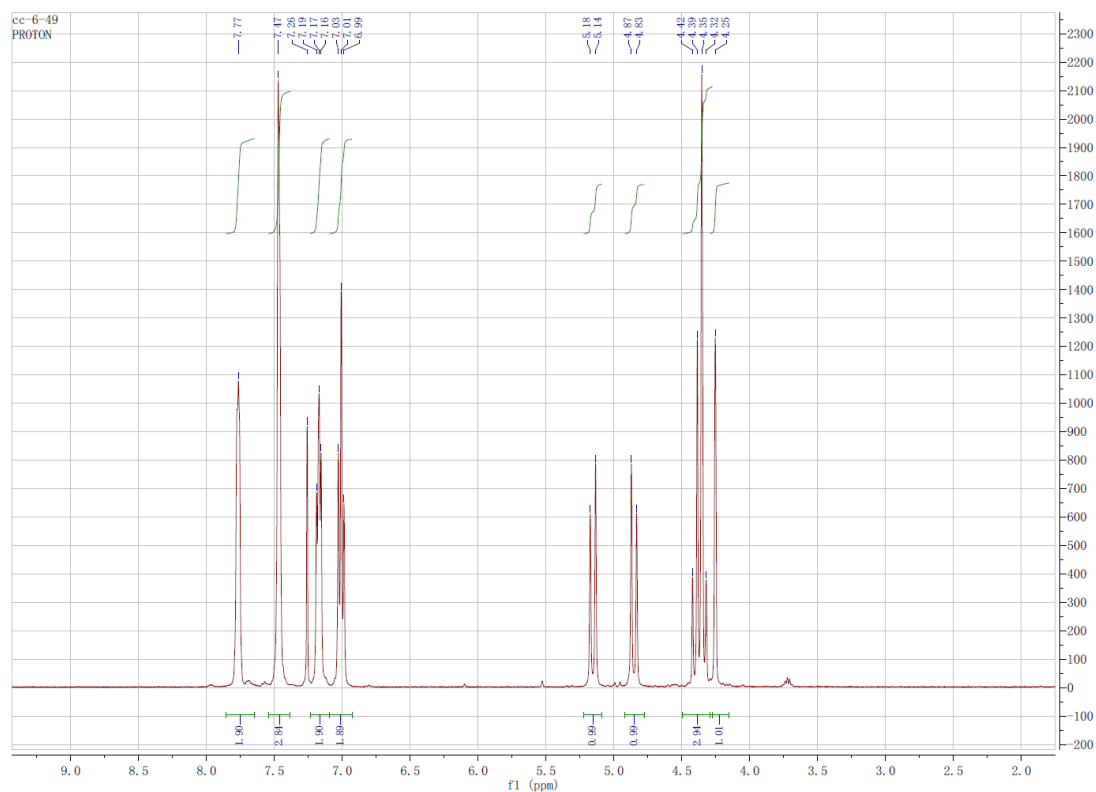
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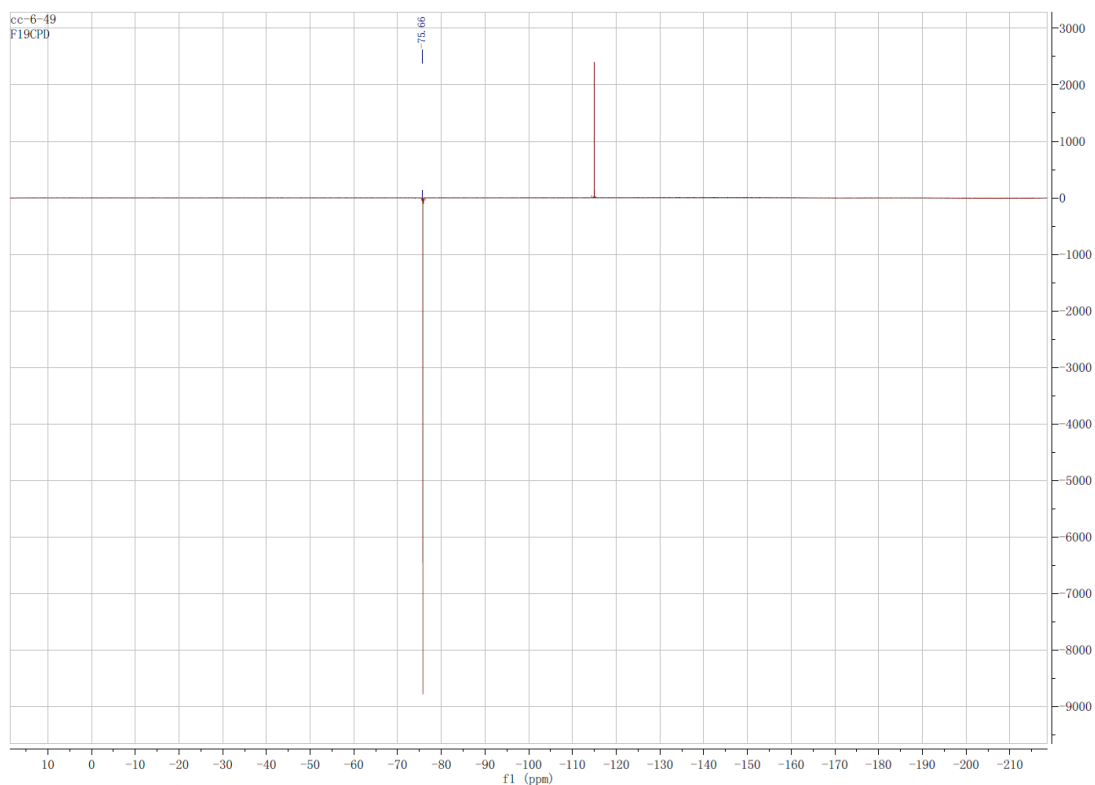
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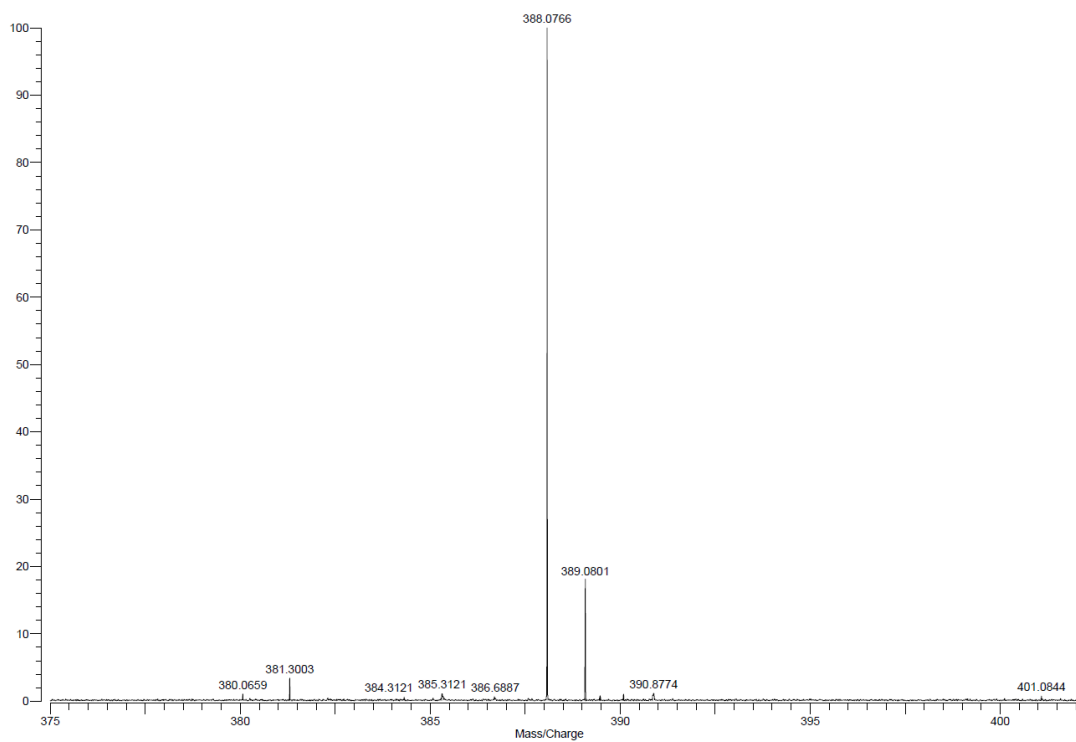




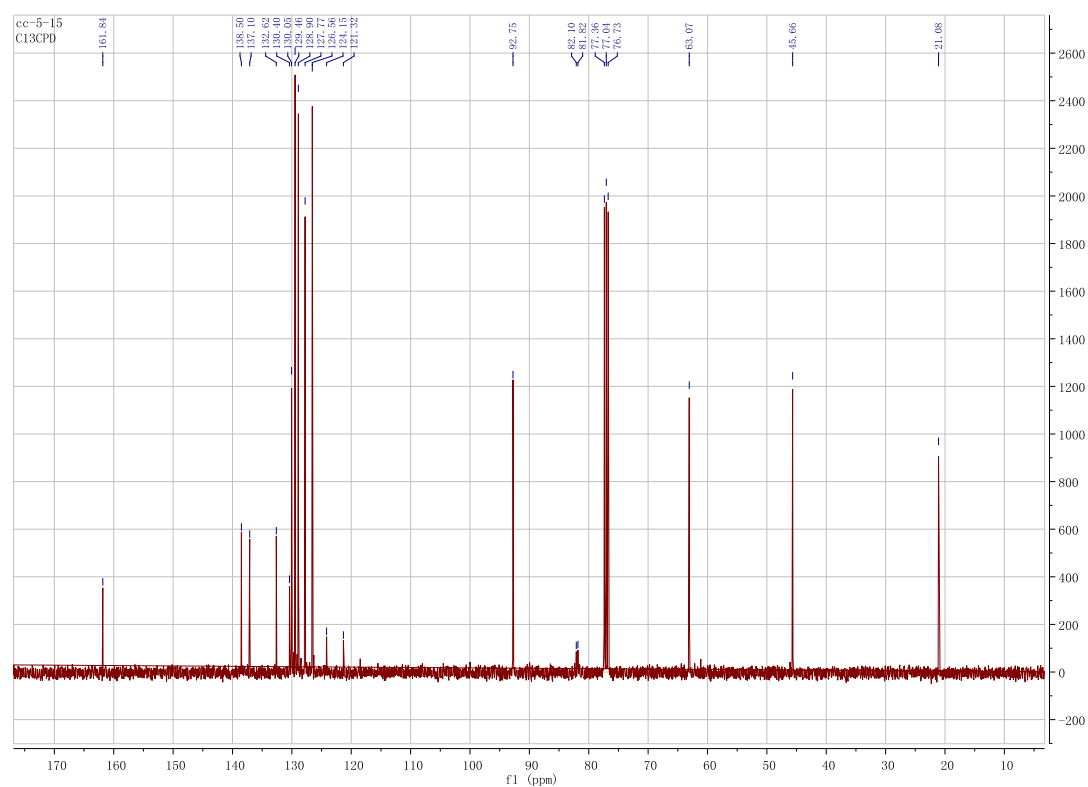
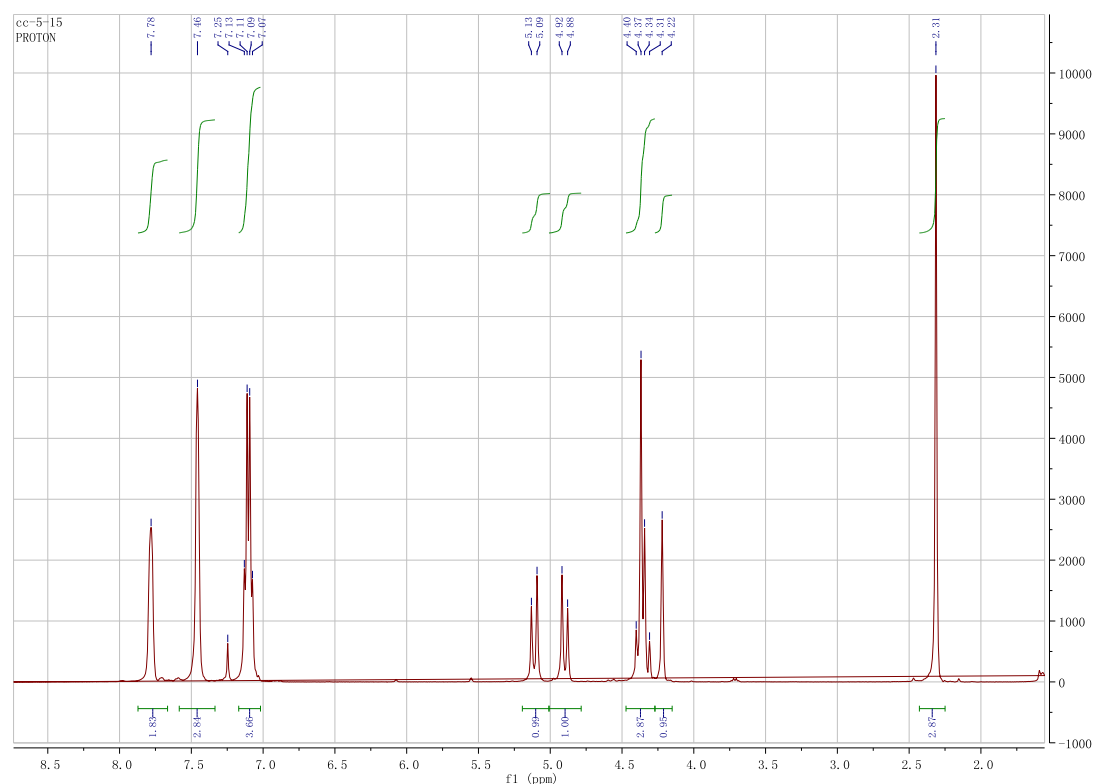
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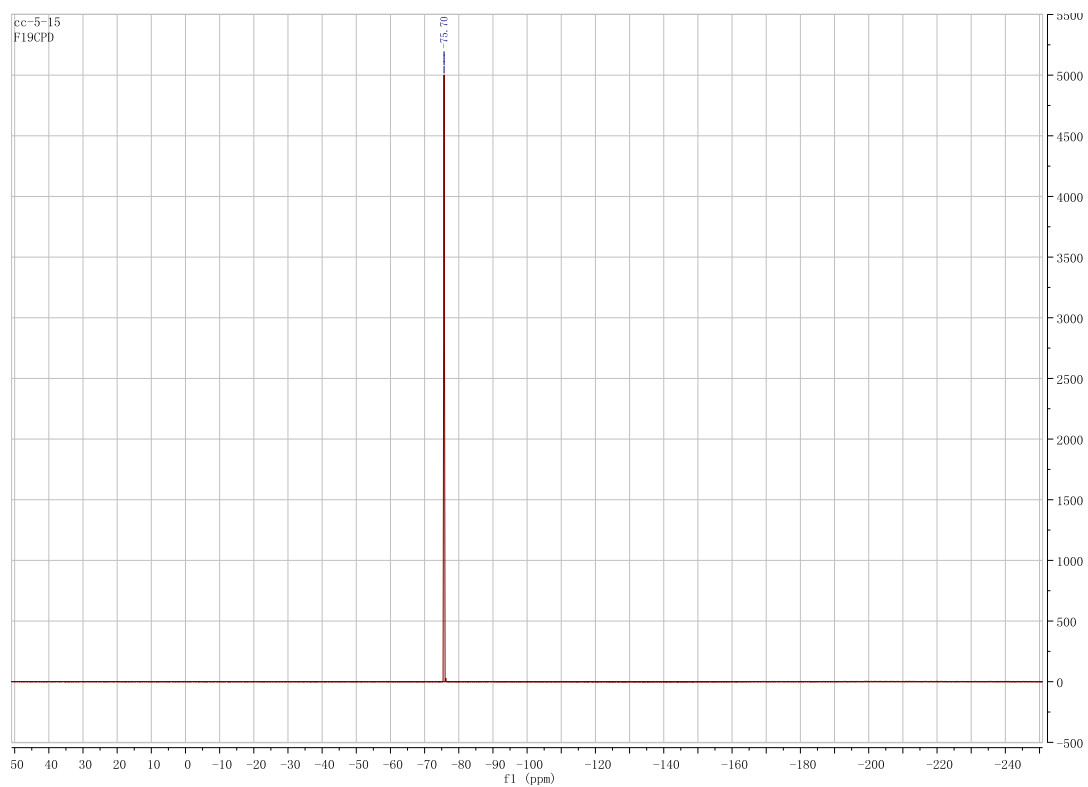
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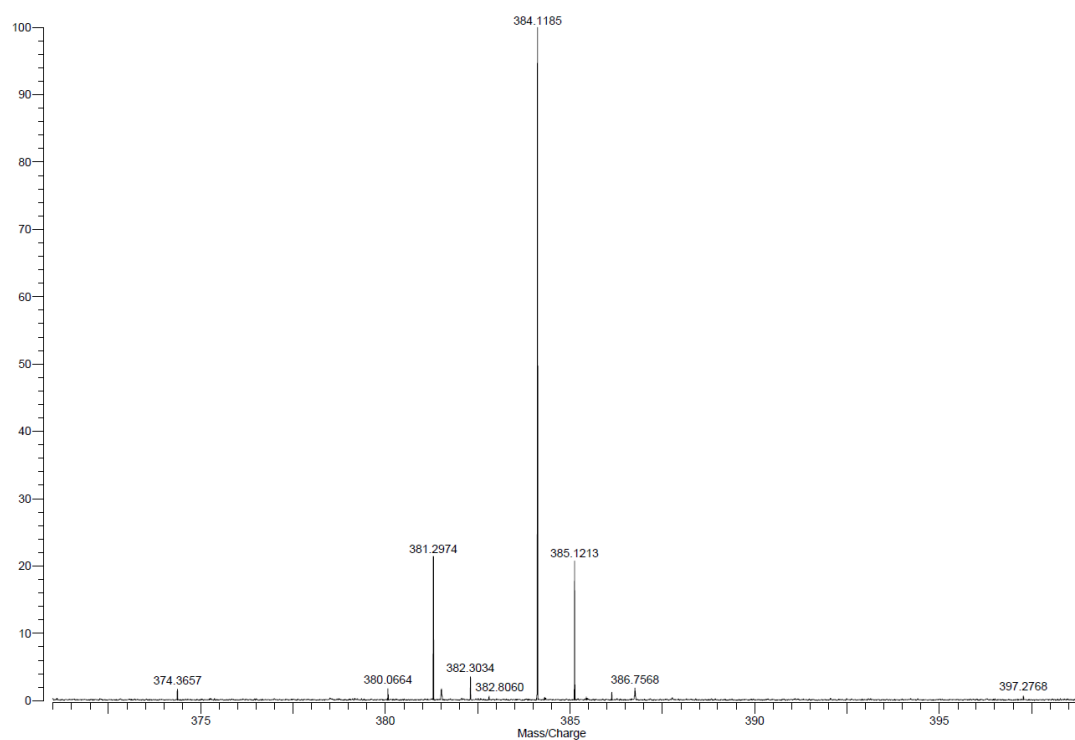
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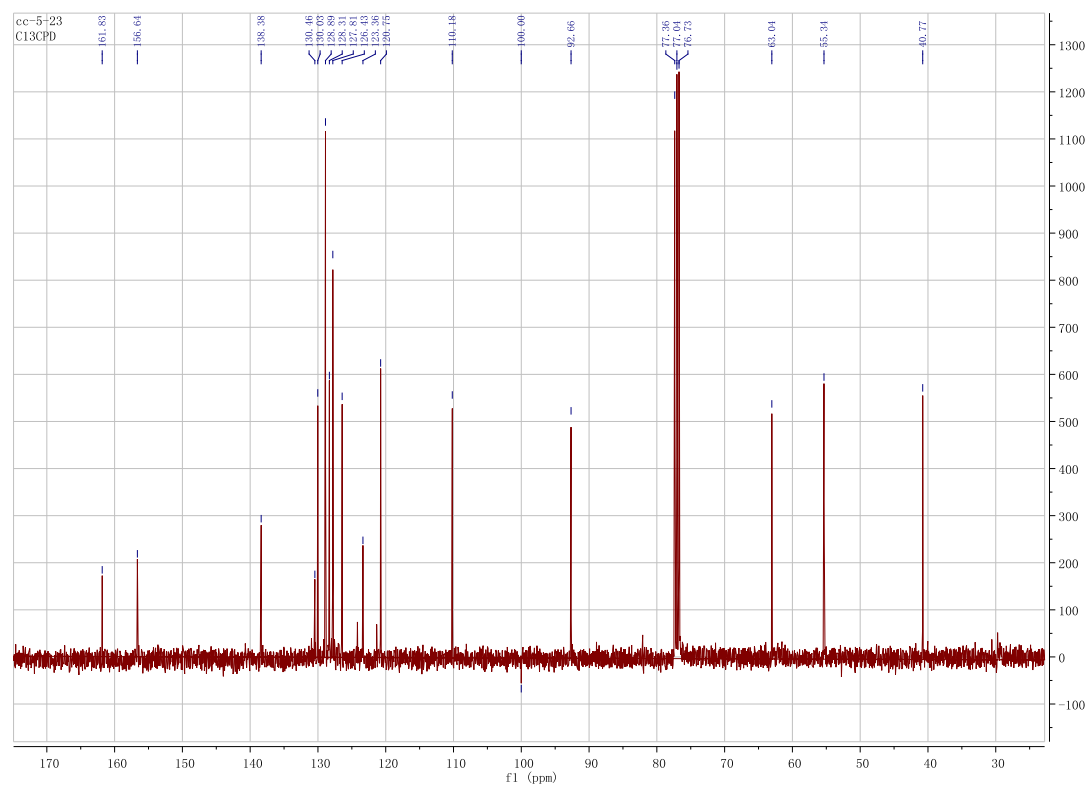
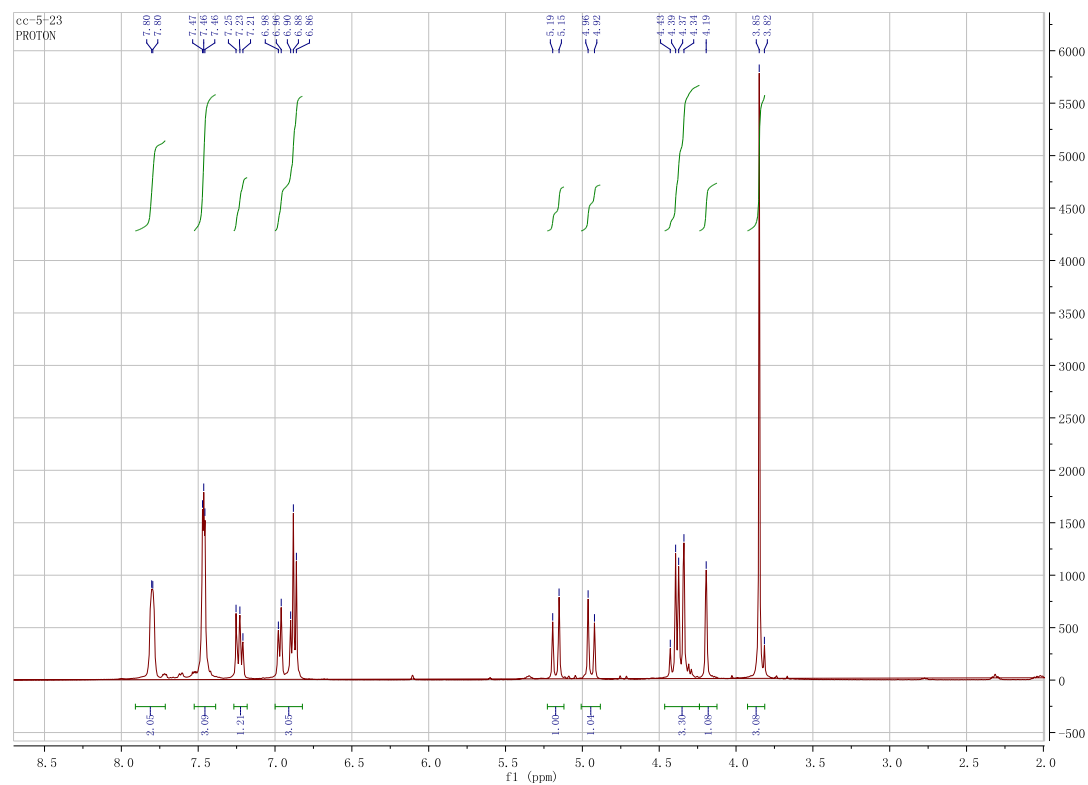


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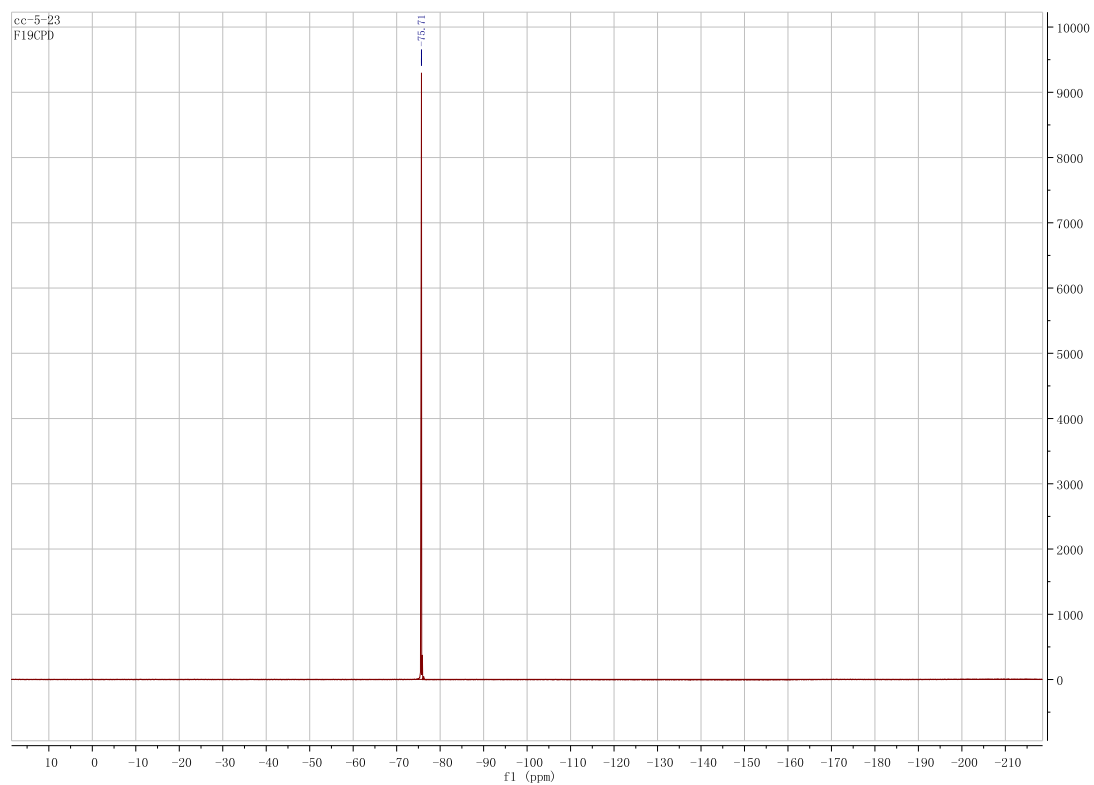
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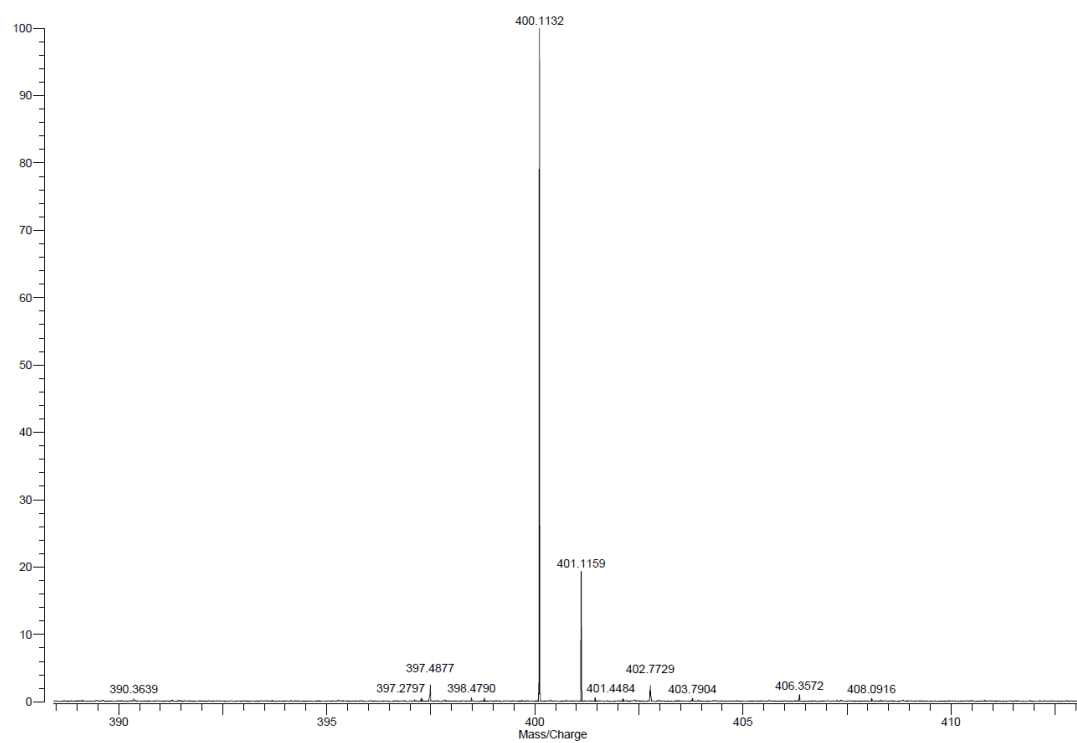




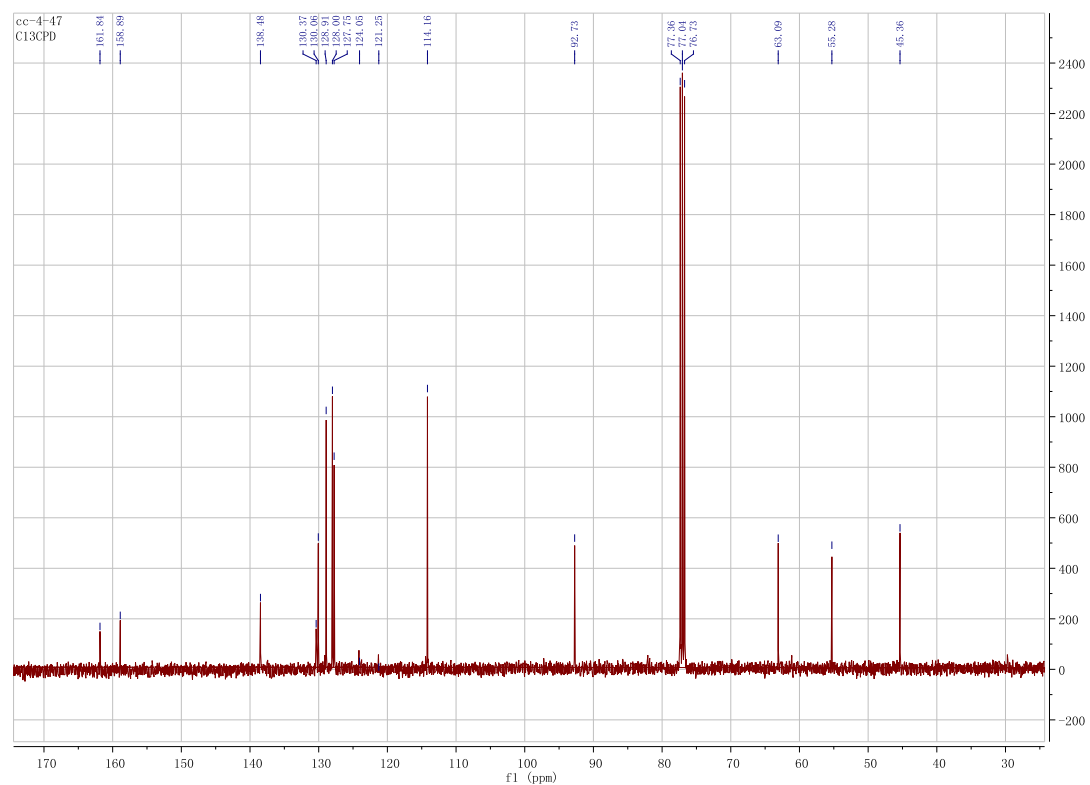
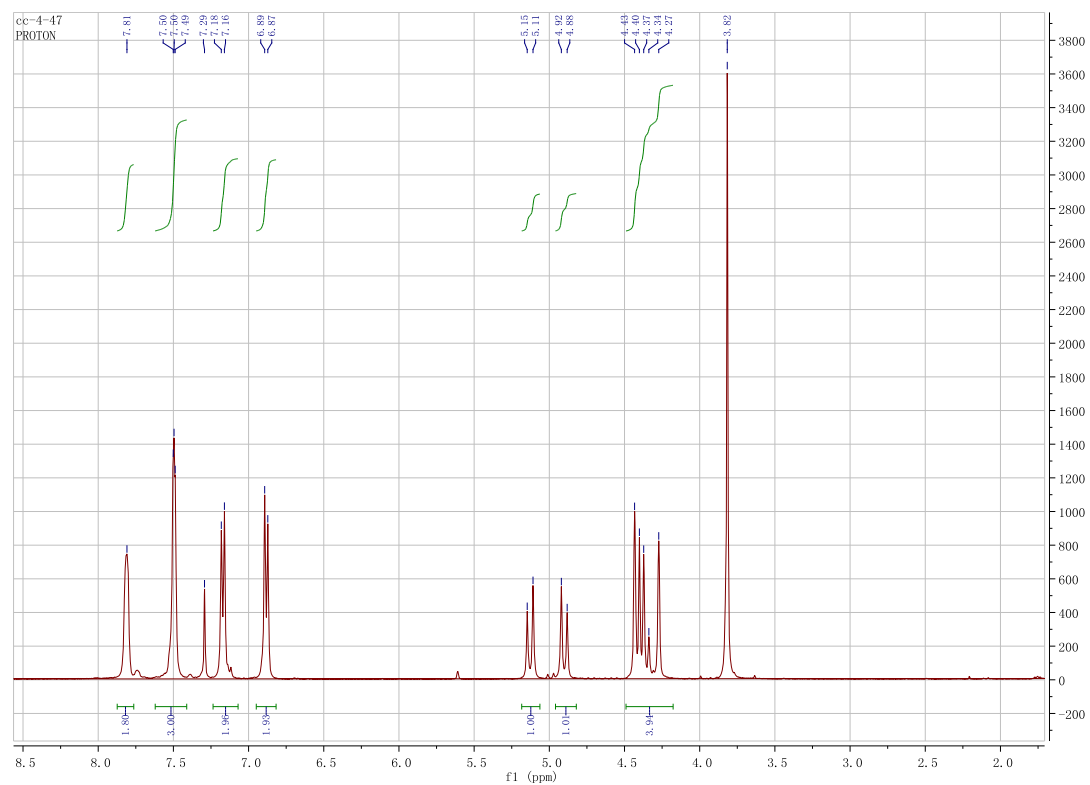
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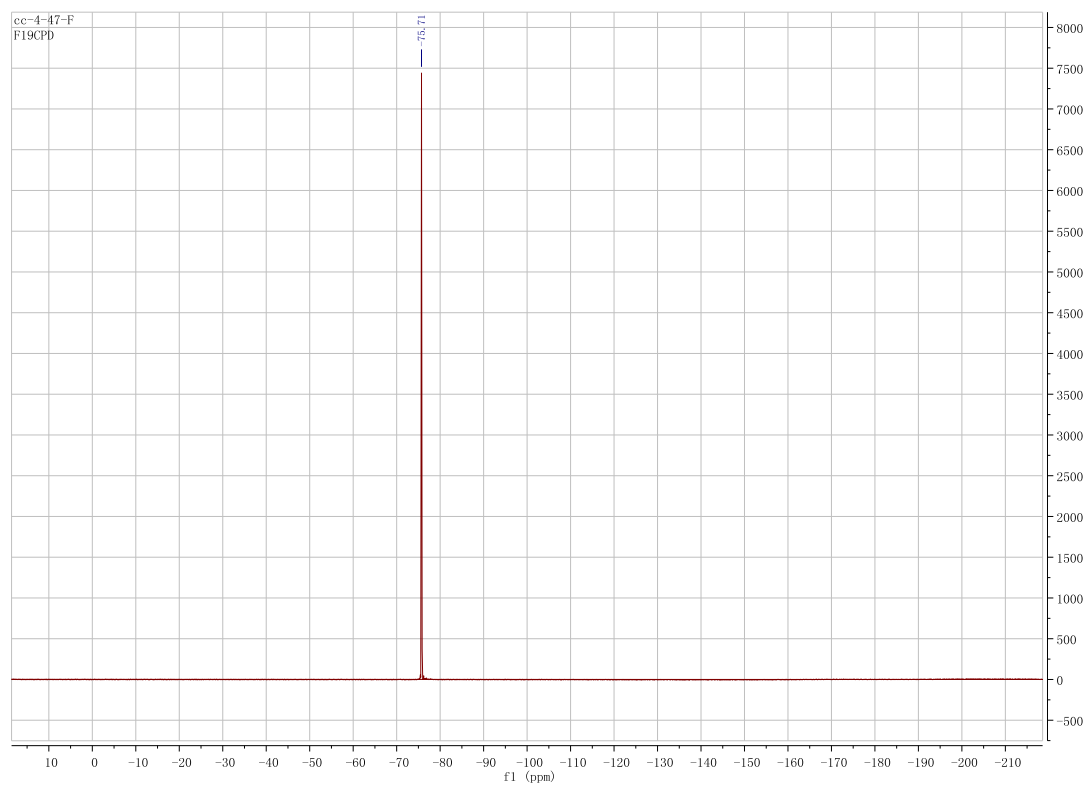
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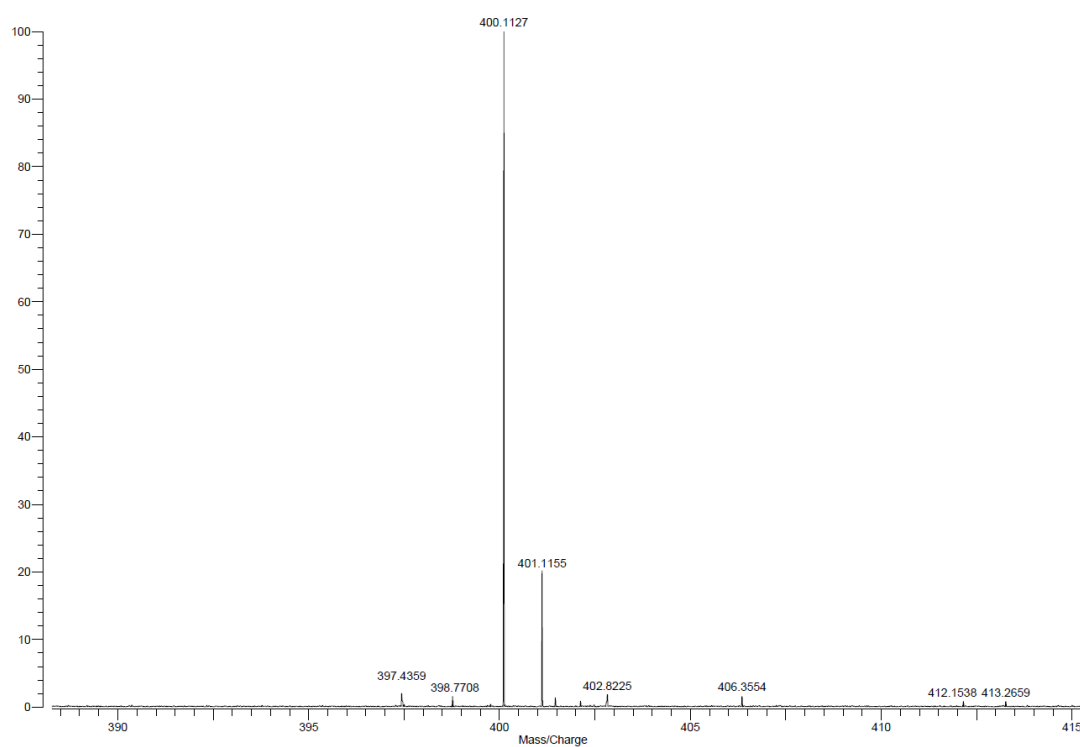




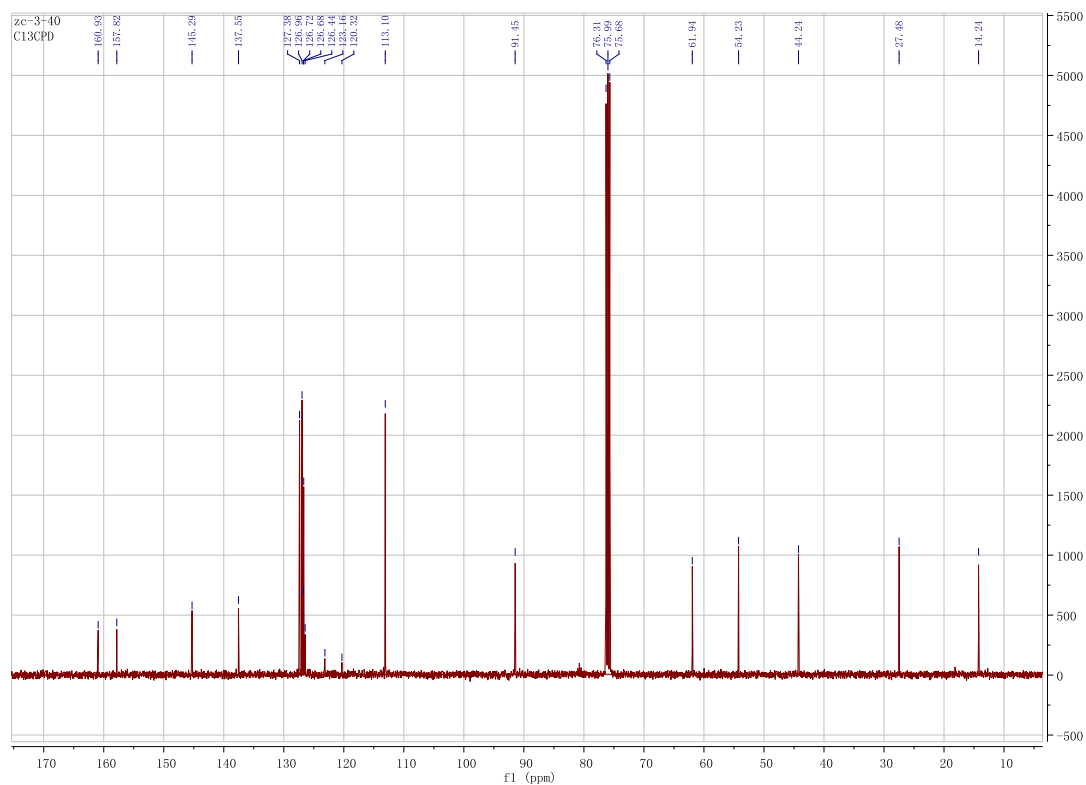
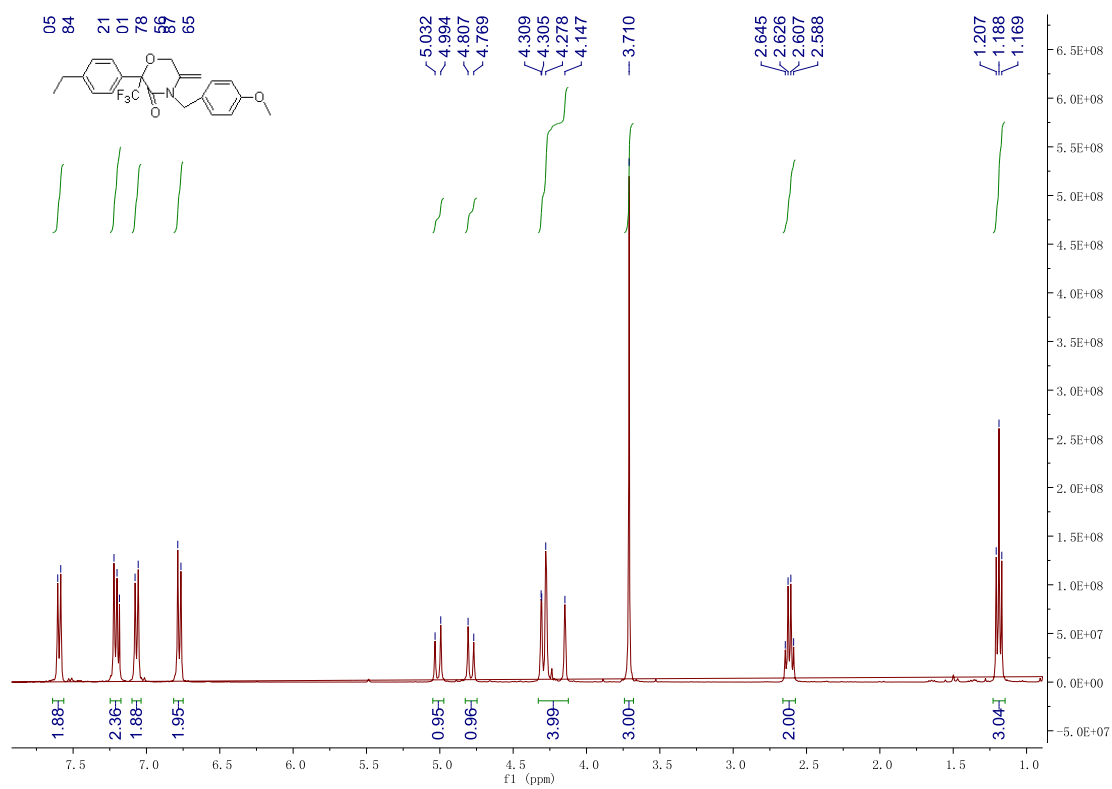
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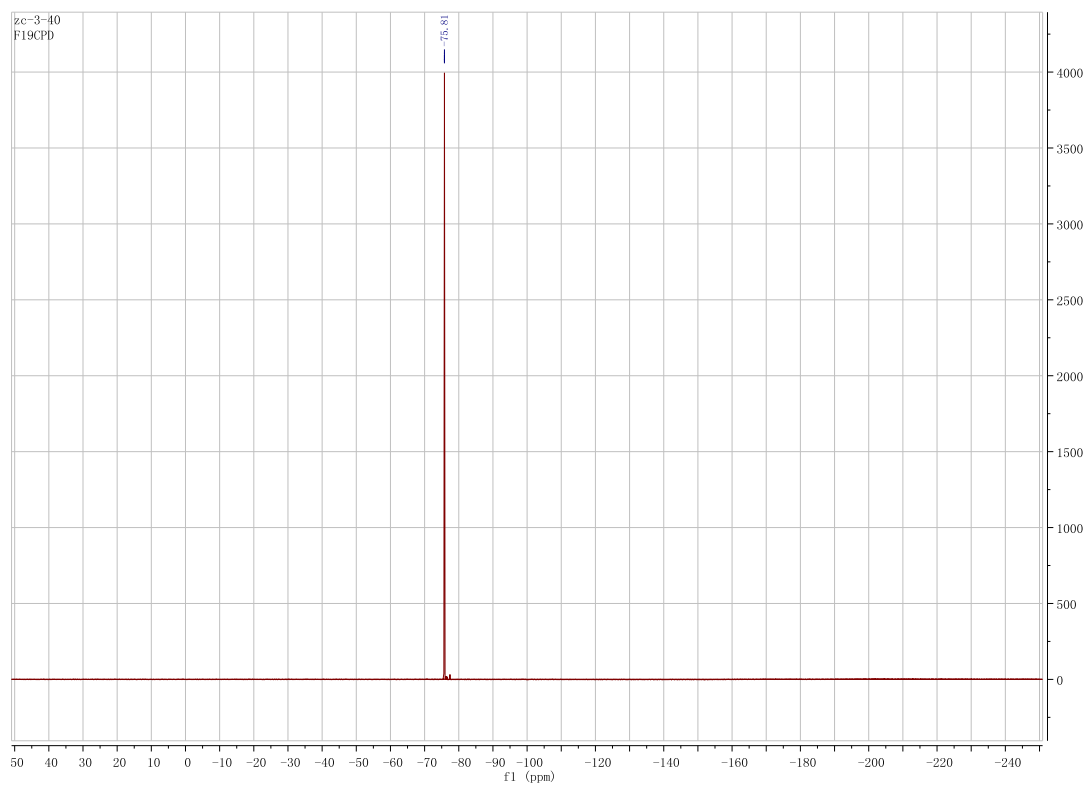
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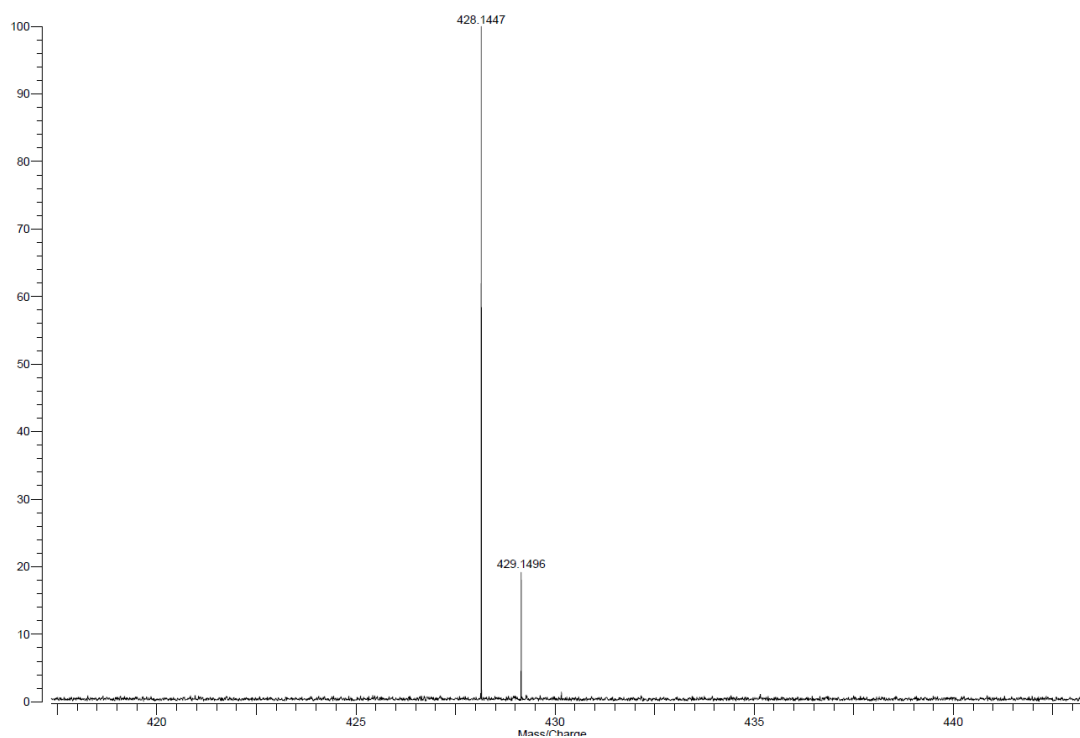
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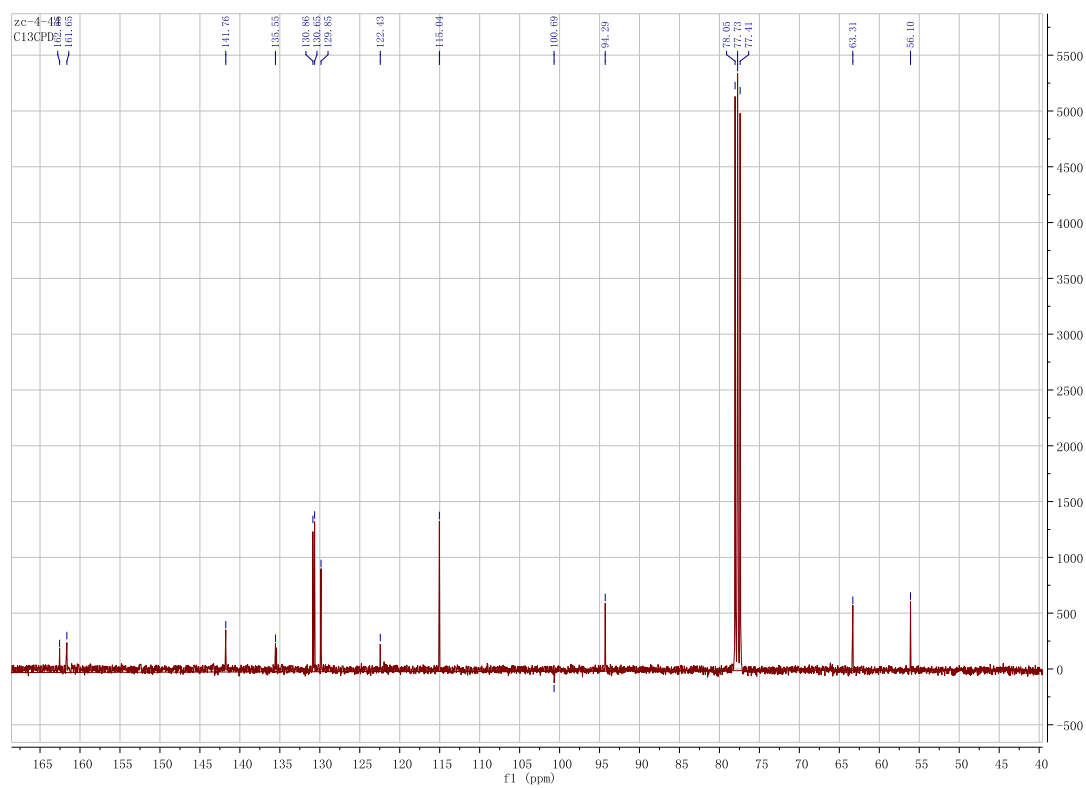
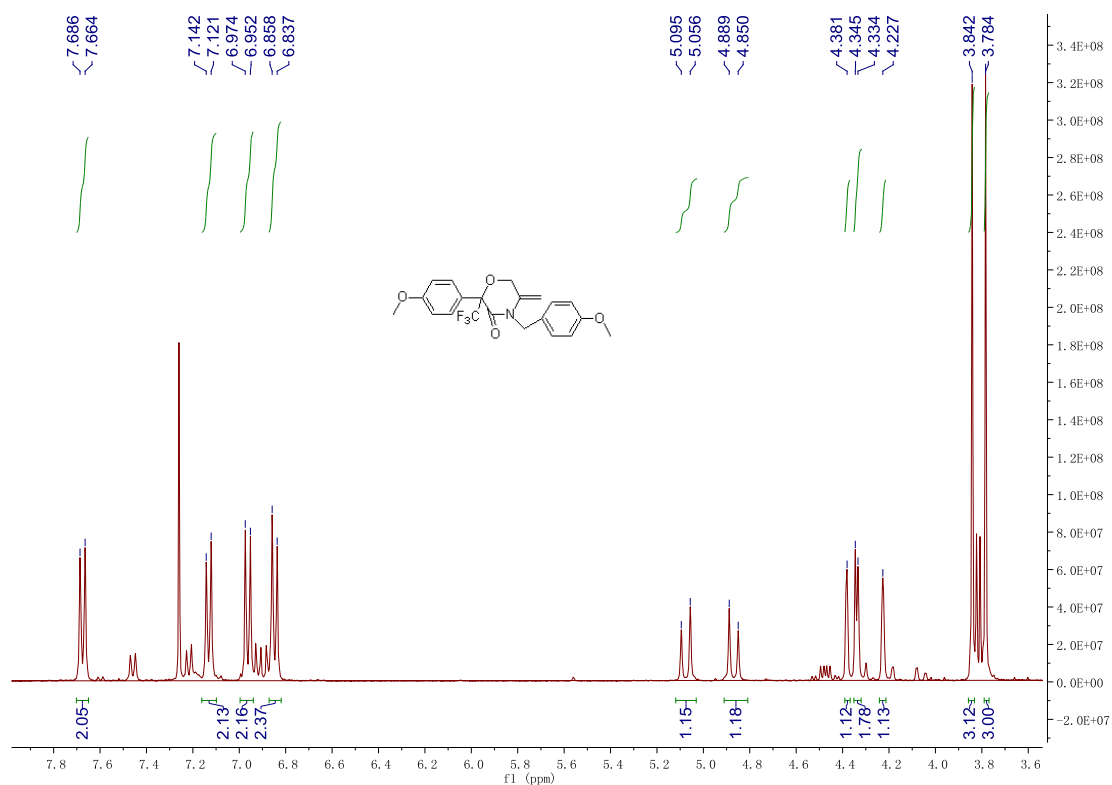


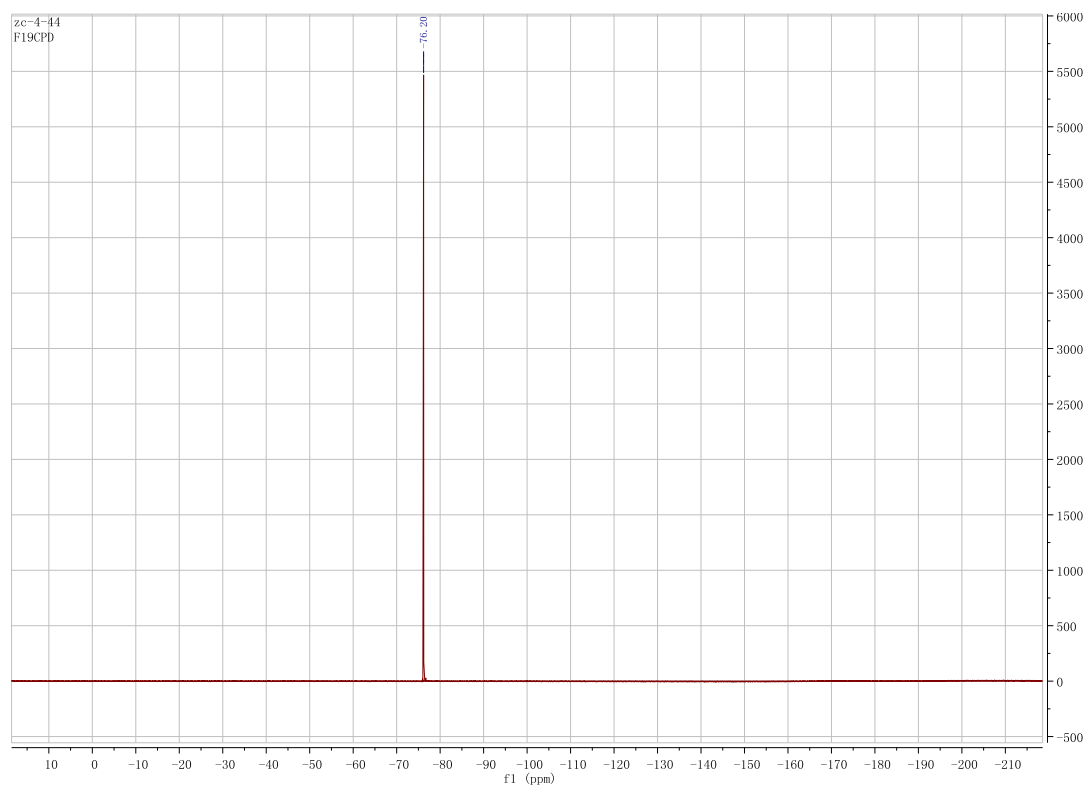
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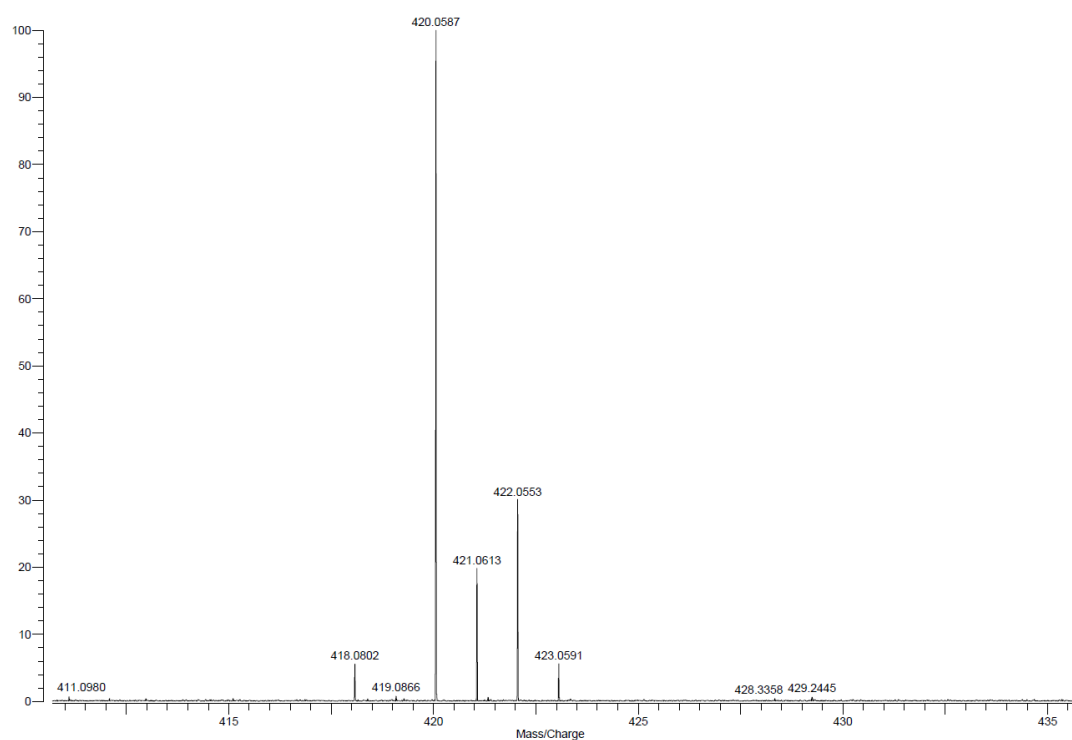




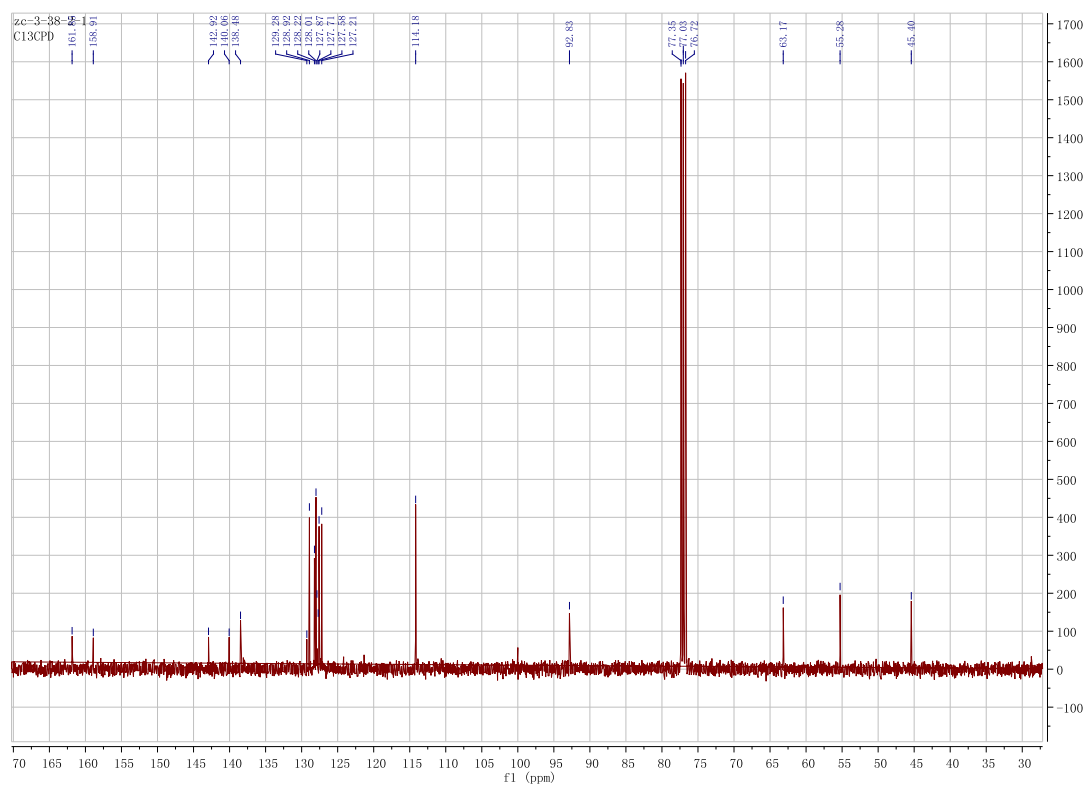
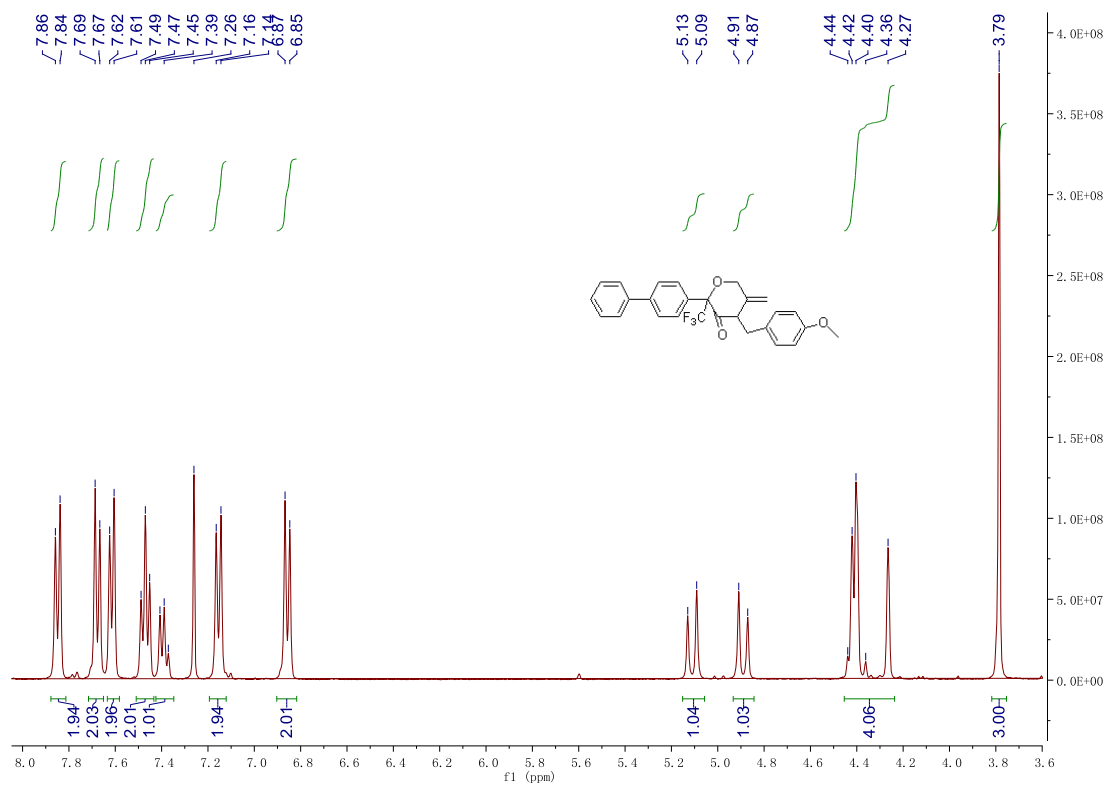
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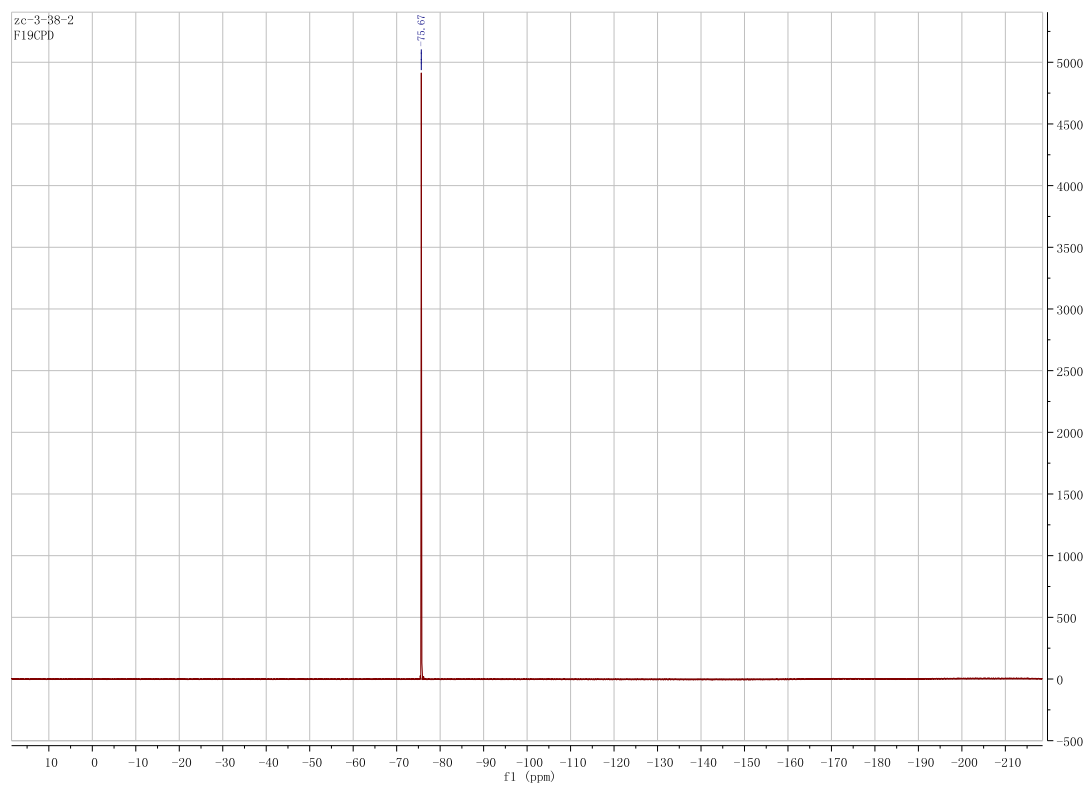
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2h

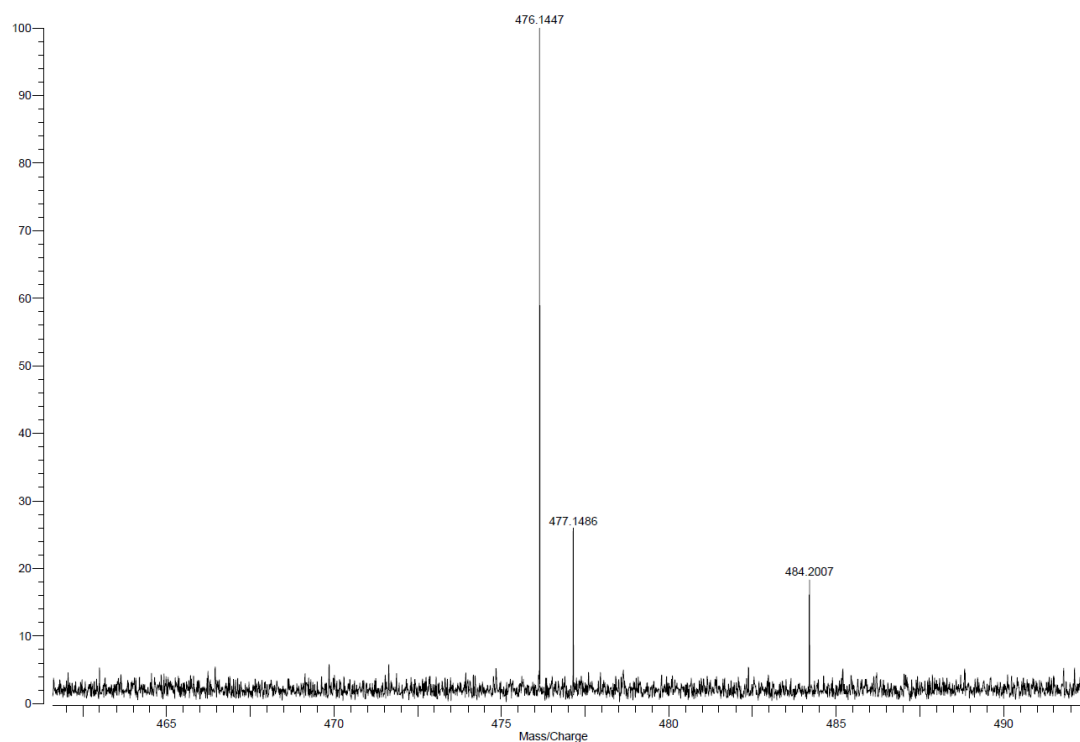




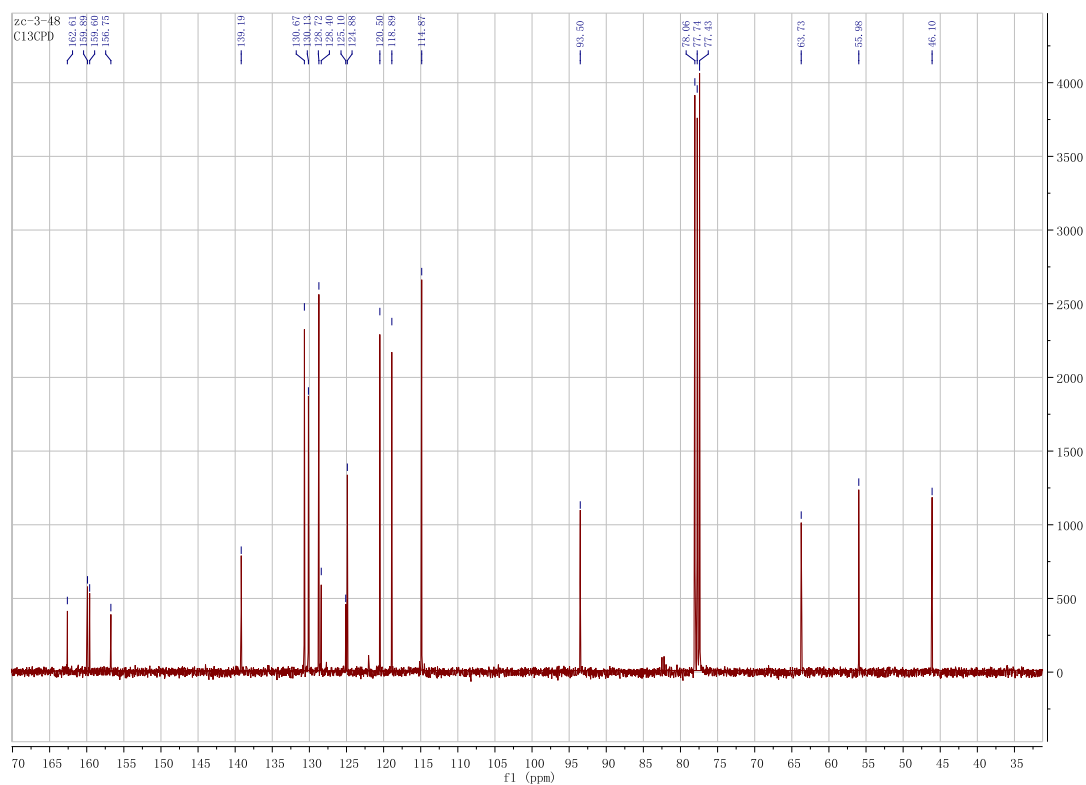
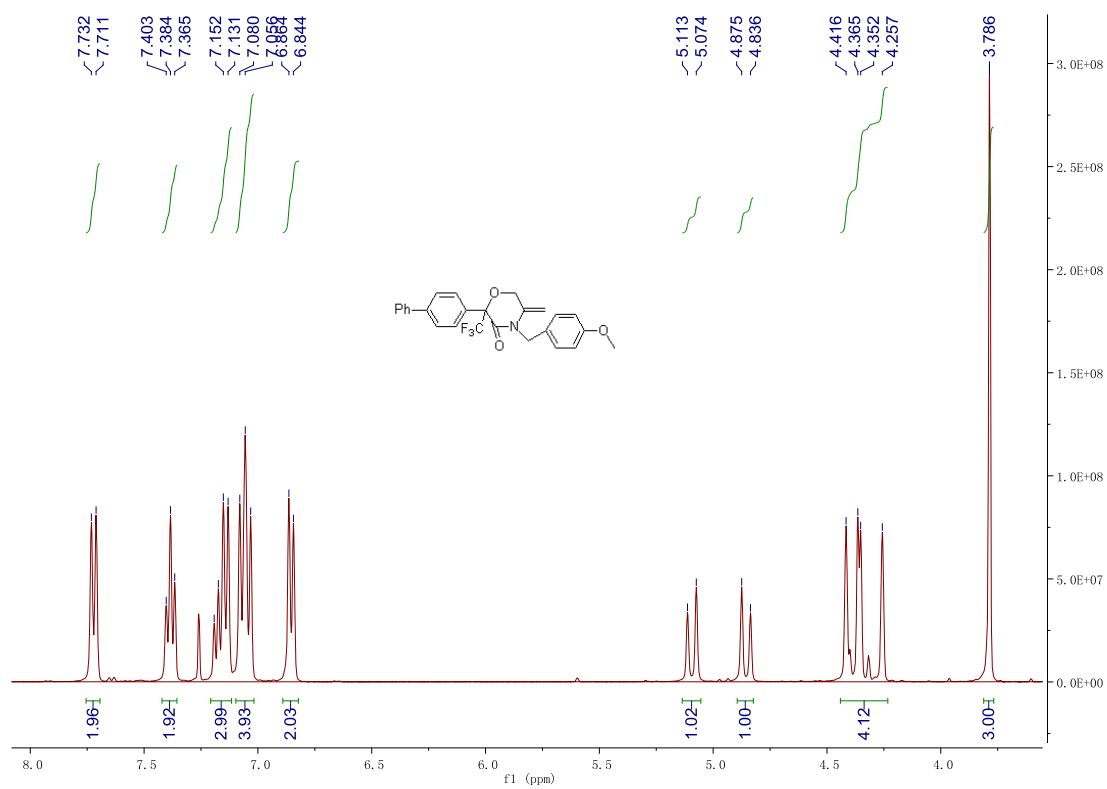


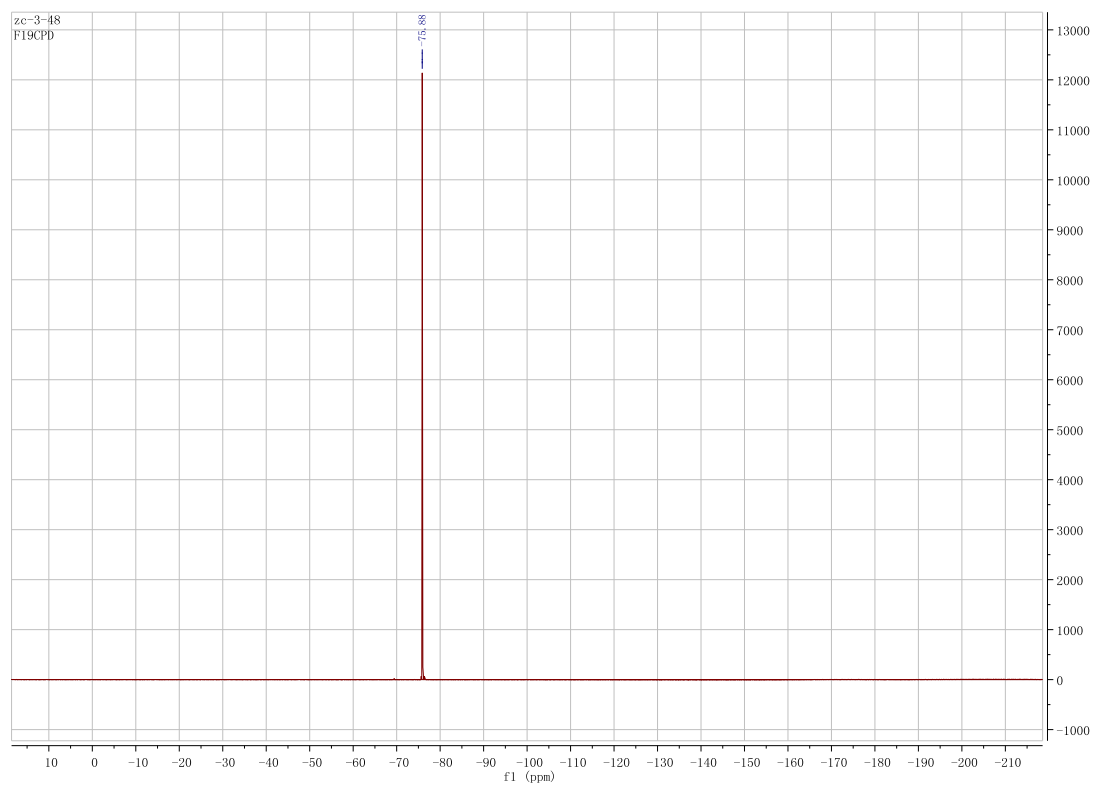
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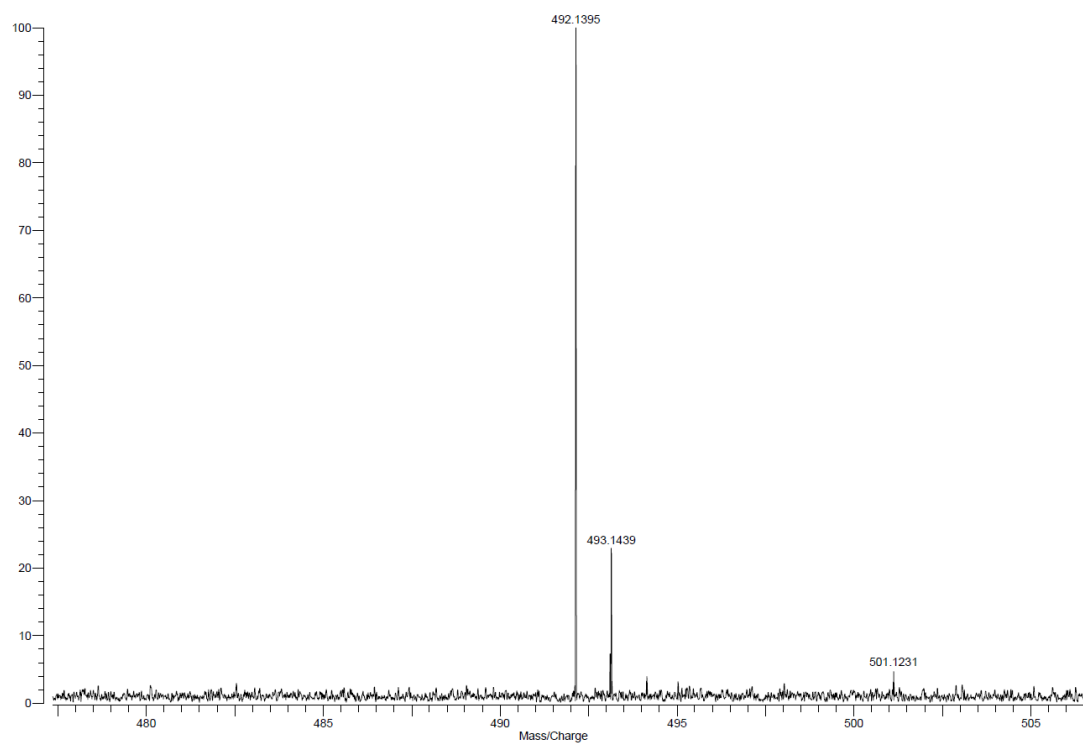




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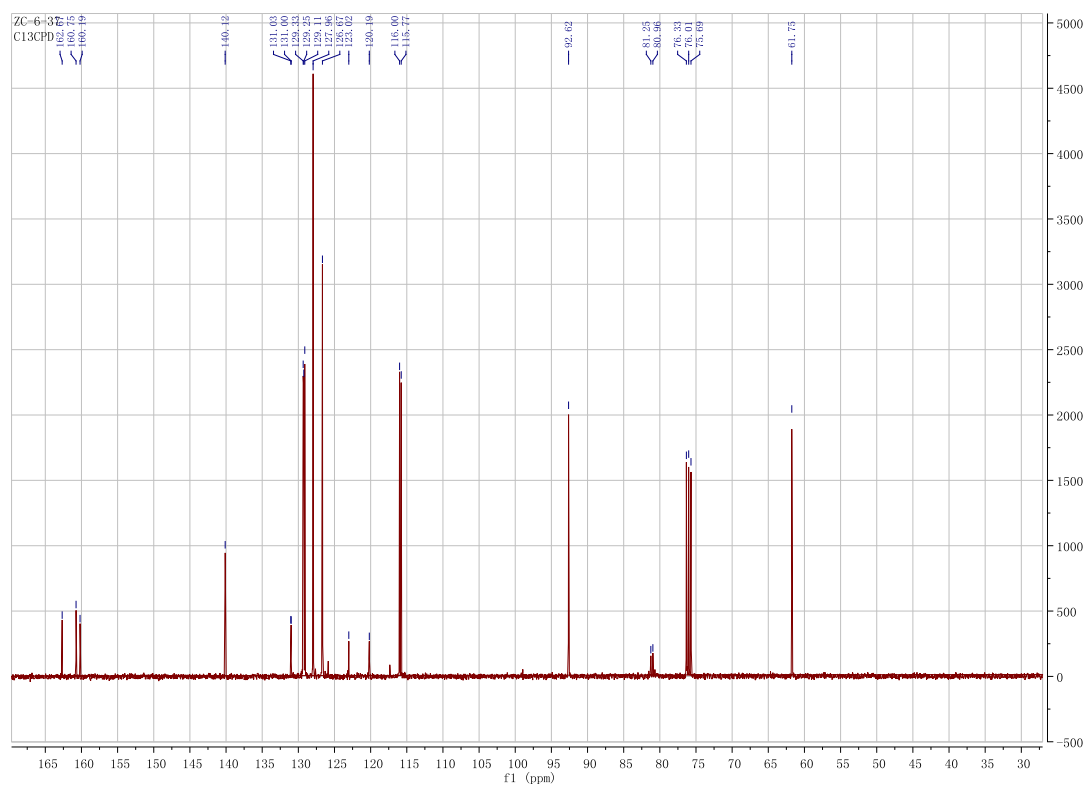
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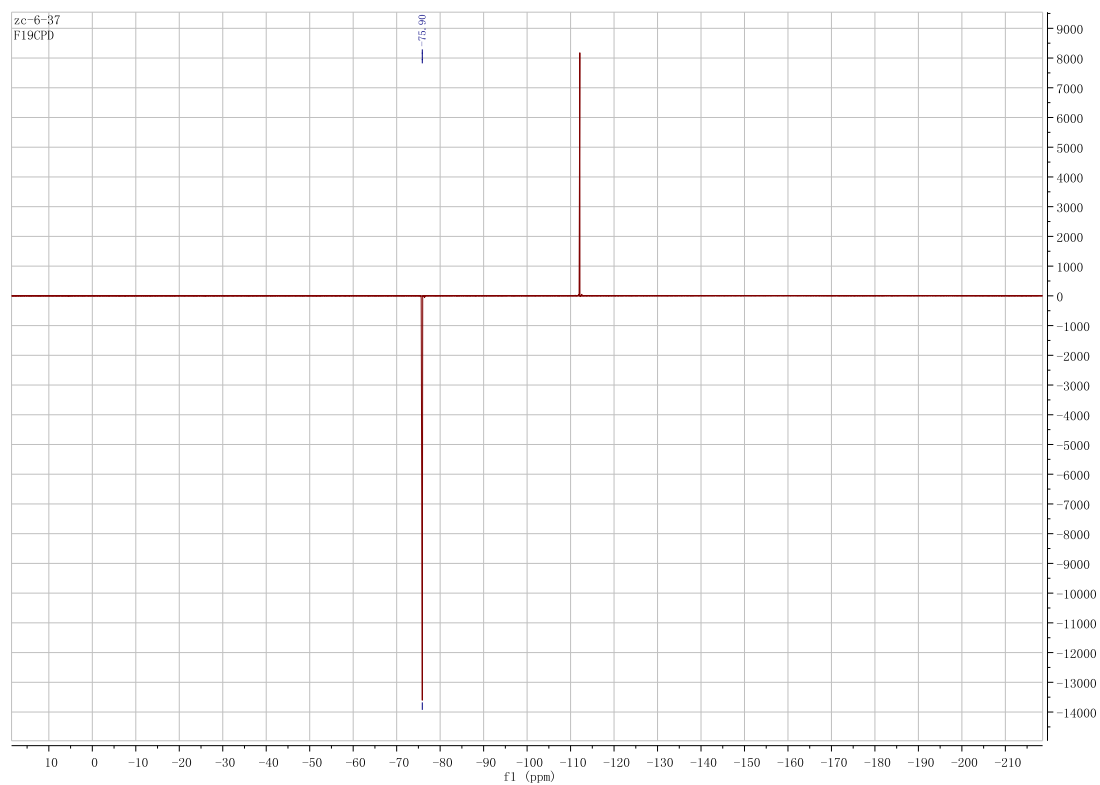


Chemical structure of compound 10 is shown above the spectrum.

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) data:

Chemical Shift (ppm)	Integration
7.808, 7.800, 7.791, 7.782	1.92
7.487, 7.480, 7.471	2.91
7.200, 7.195, 7.181	3.82
7.26 (solvent)	-
4.565, 4.531, 4.497, 4.462	2.02
4.237	1.00
3.858, 3.854	0.98

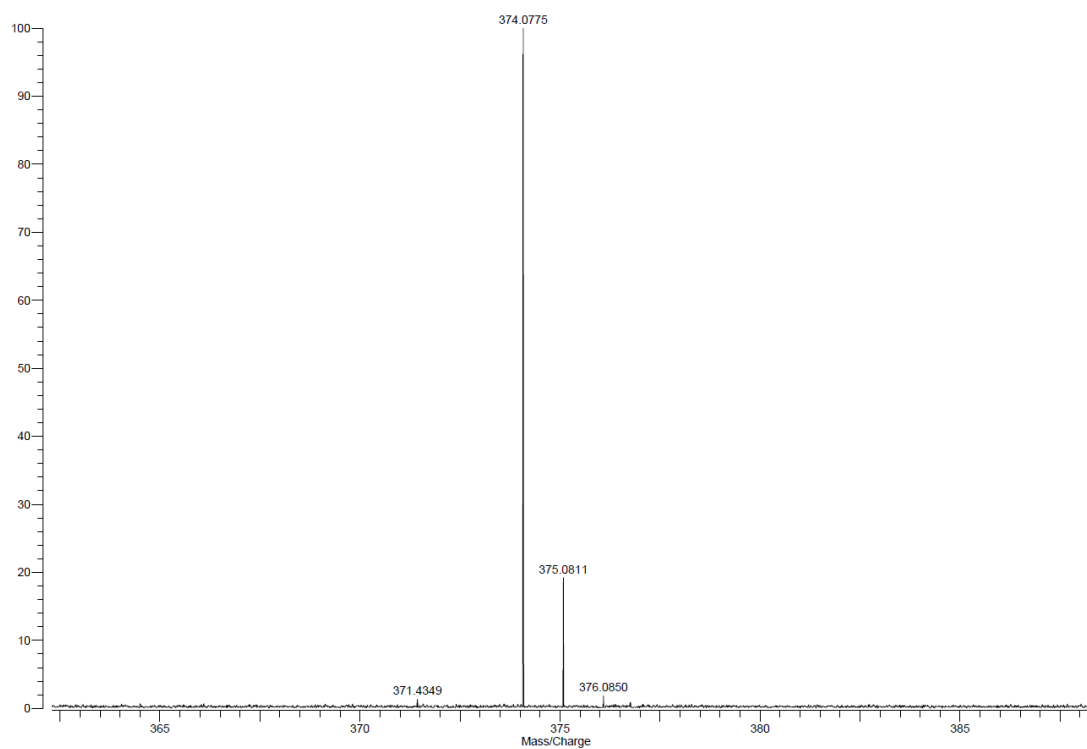




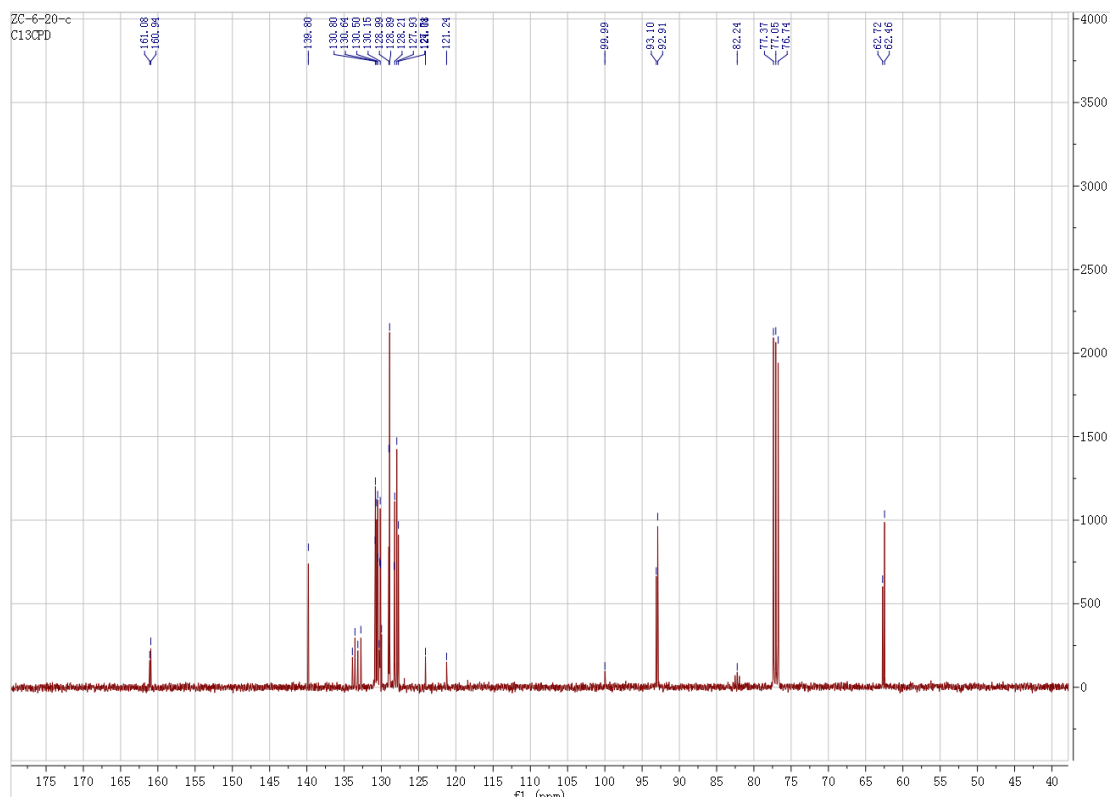
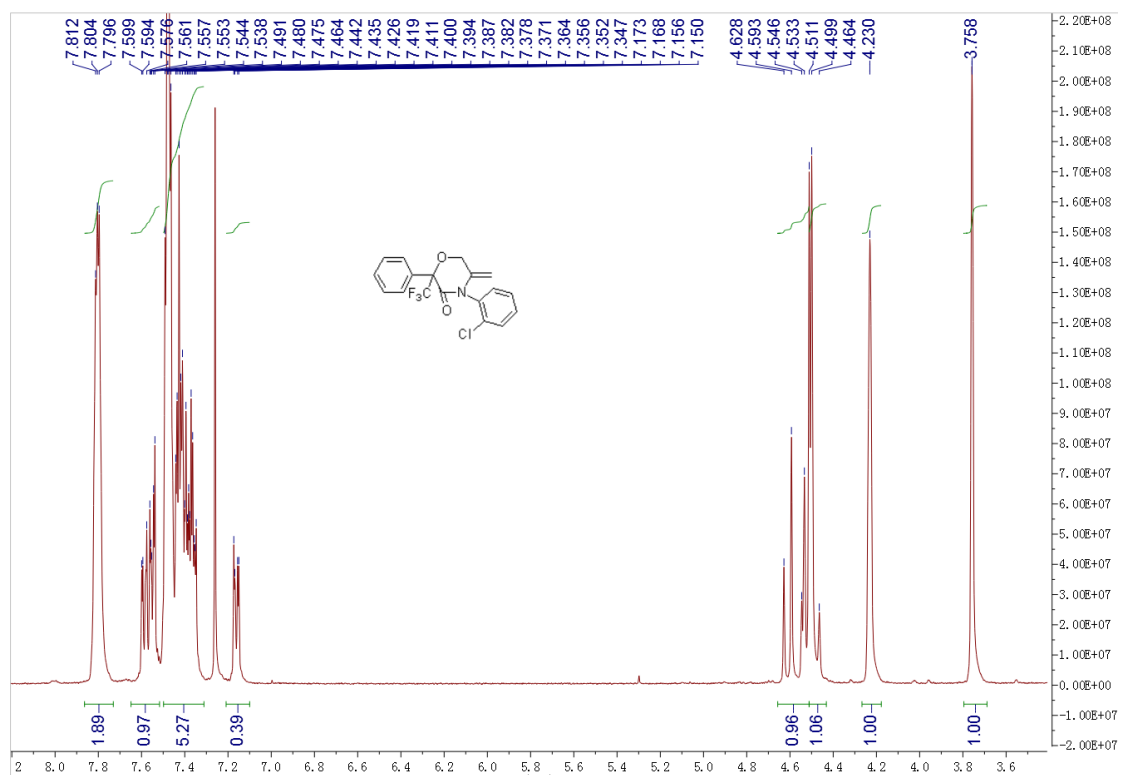
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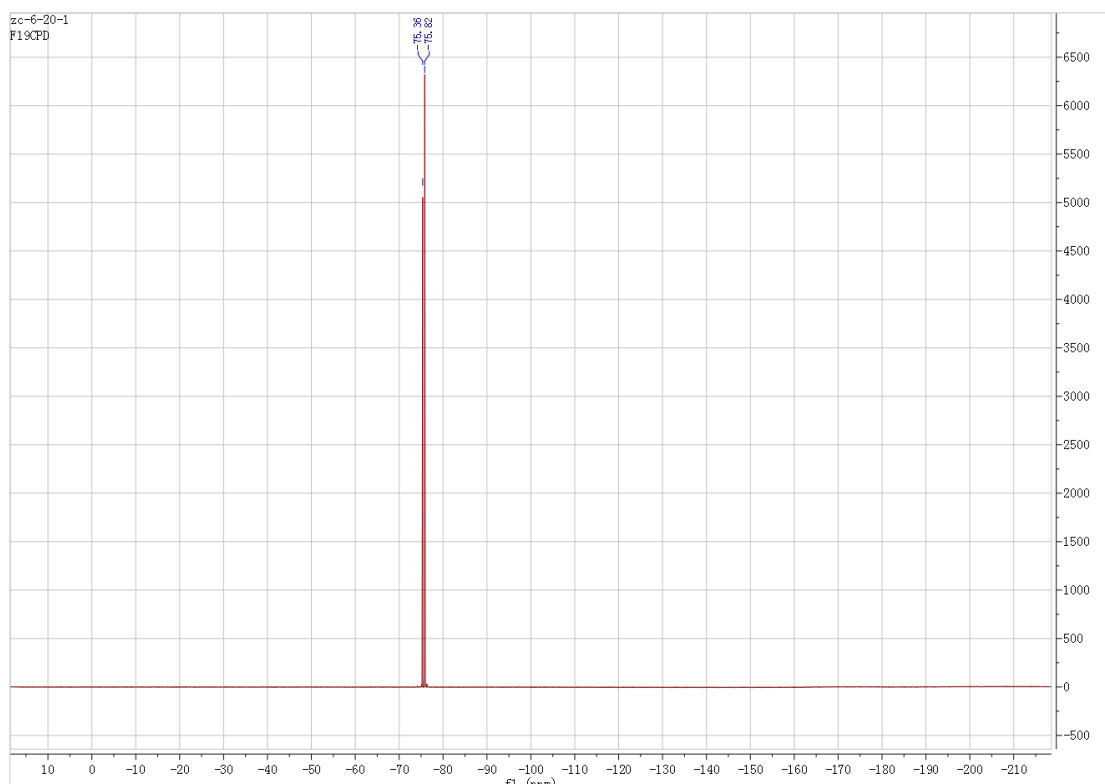
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3b

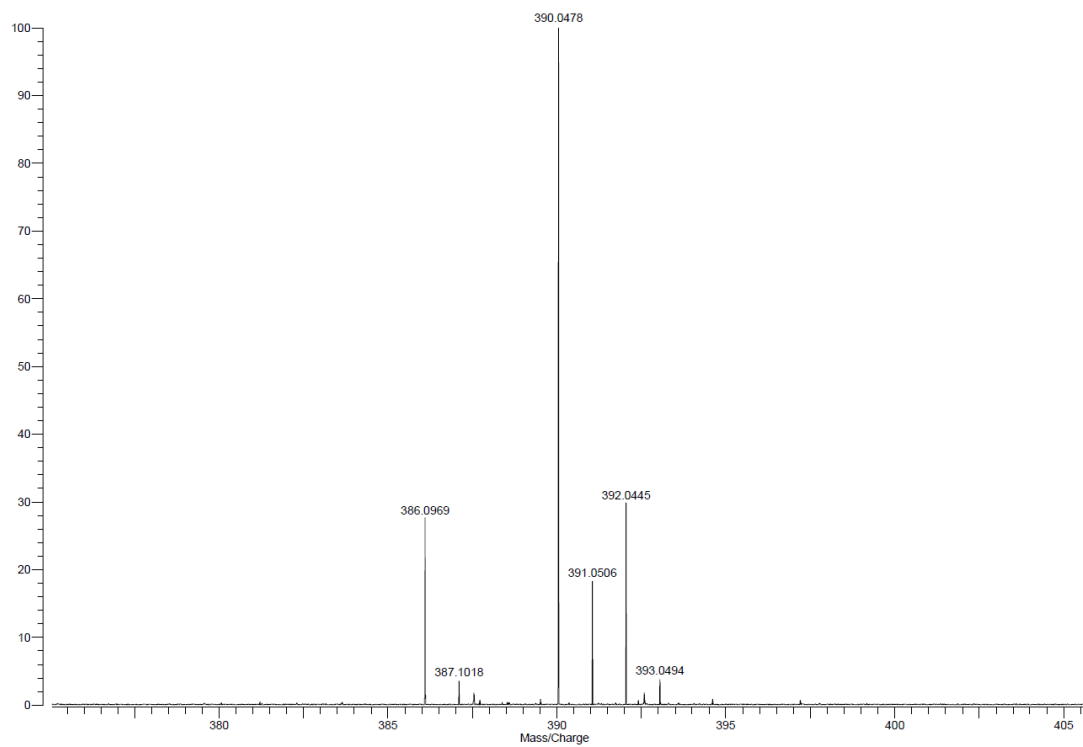




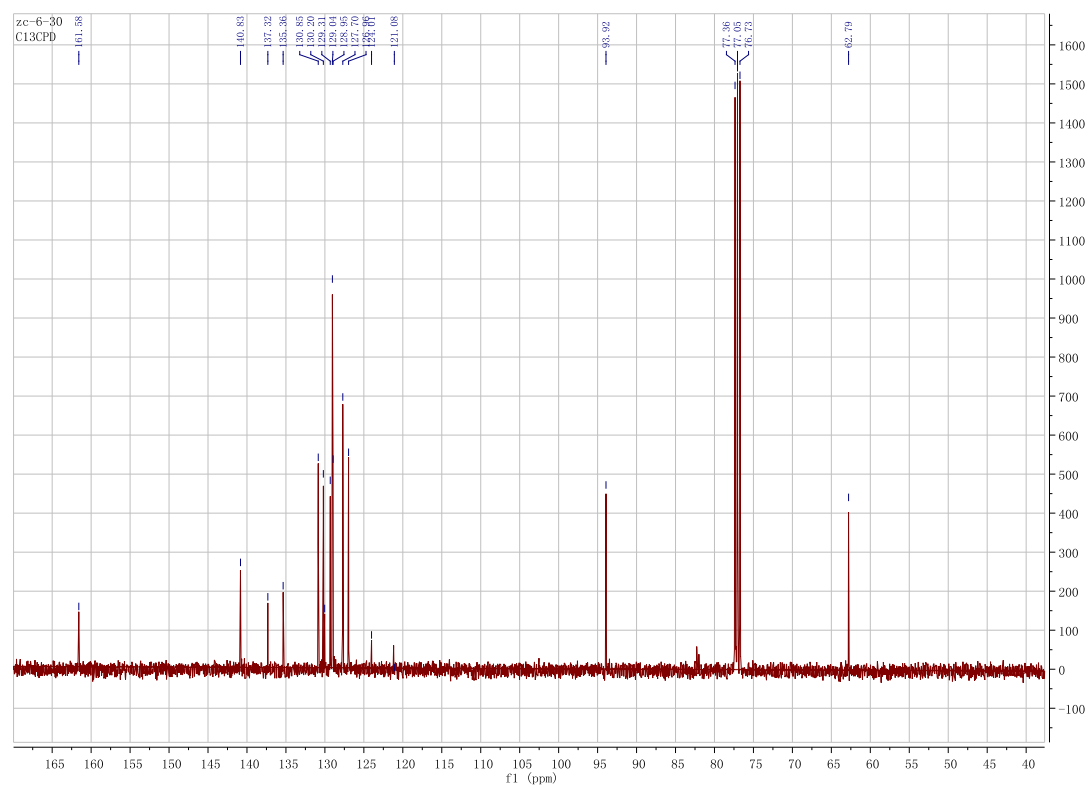
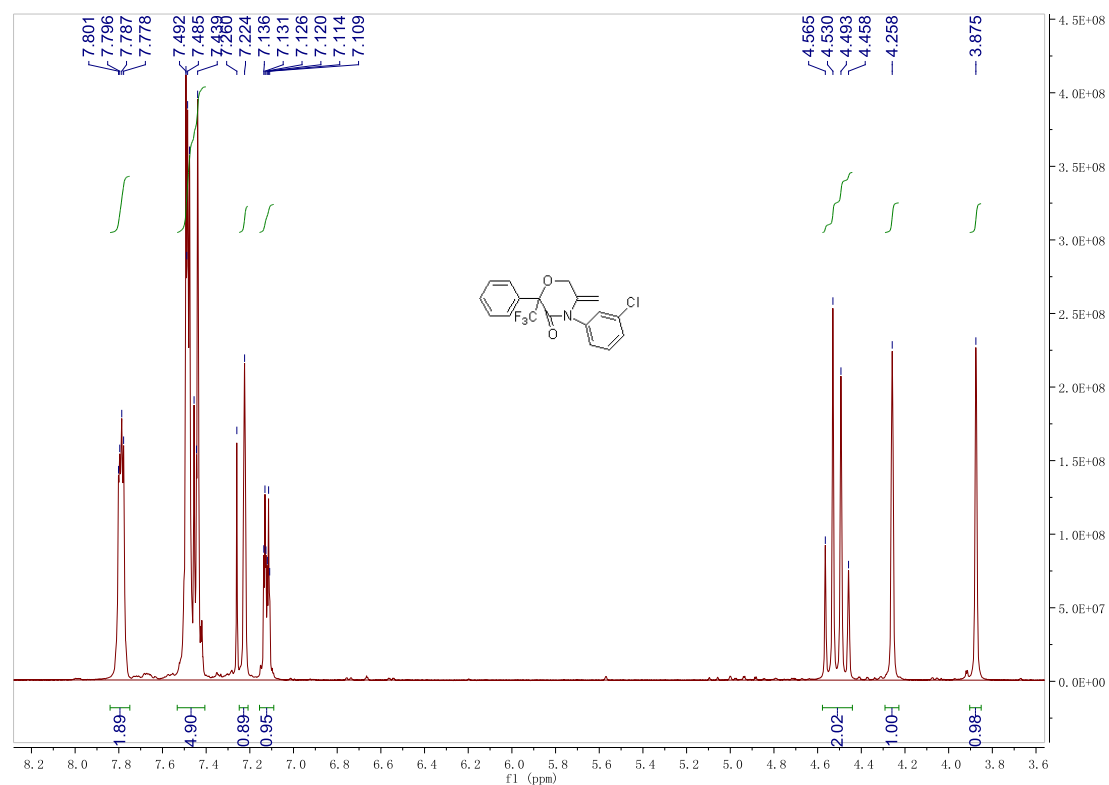
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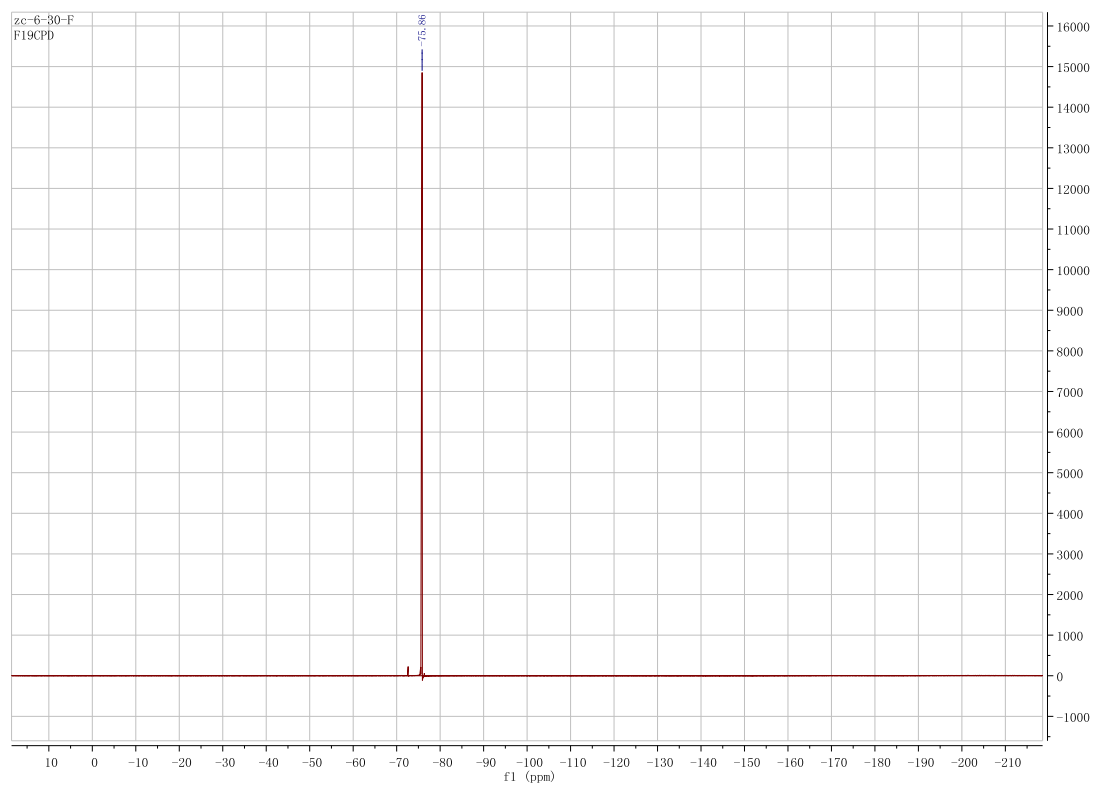
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3c



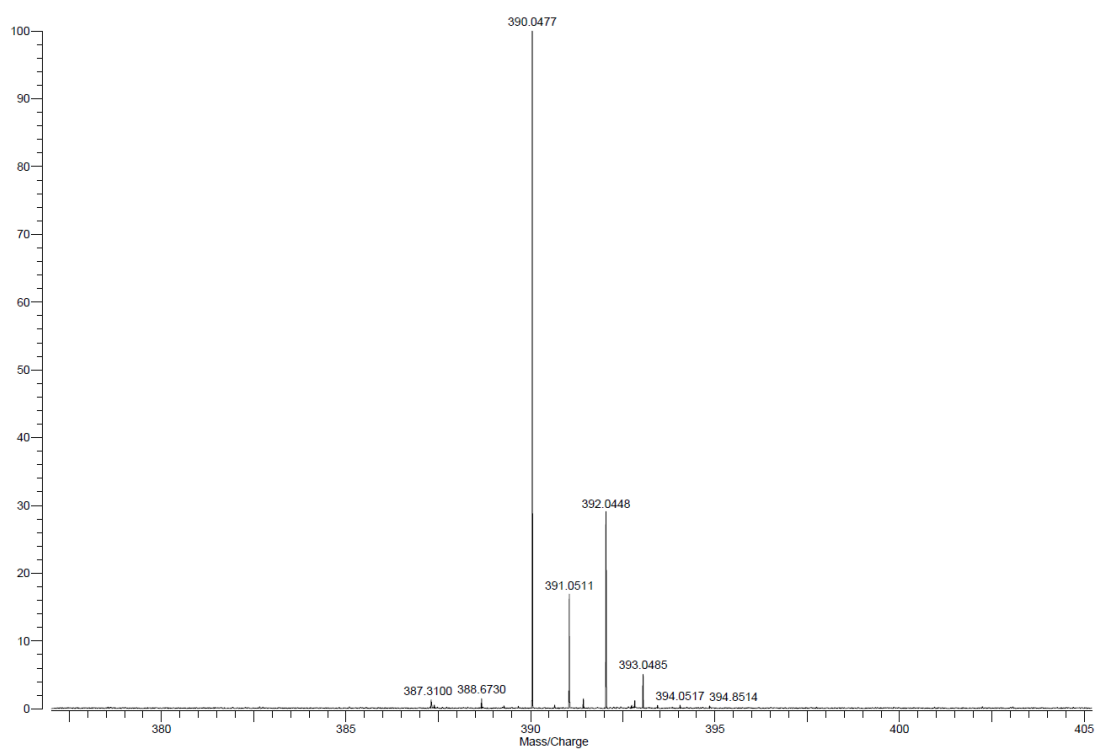




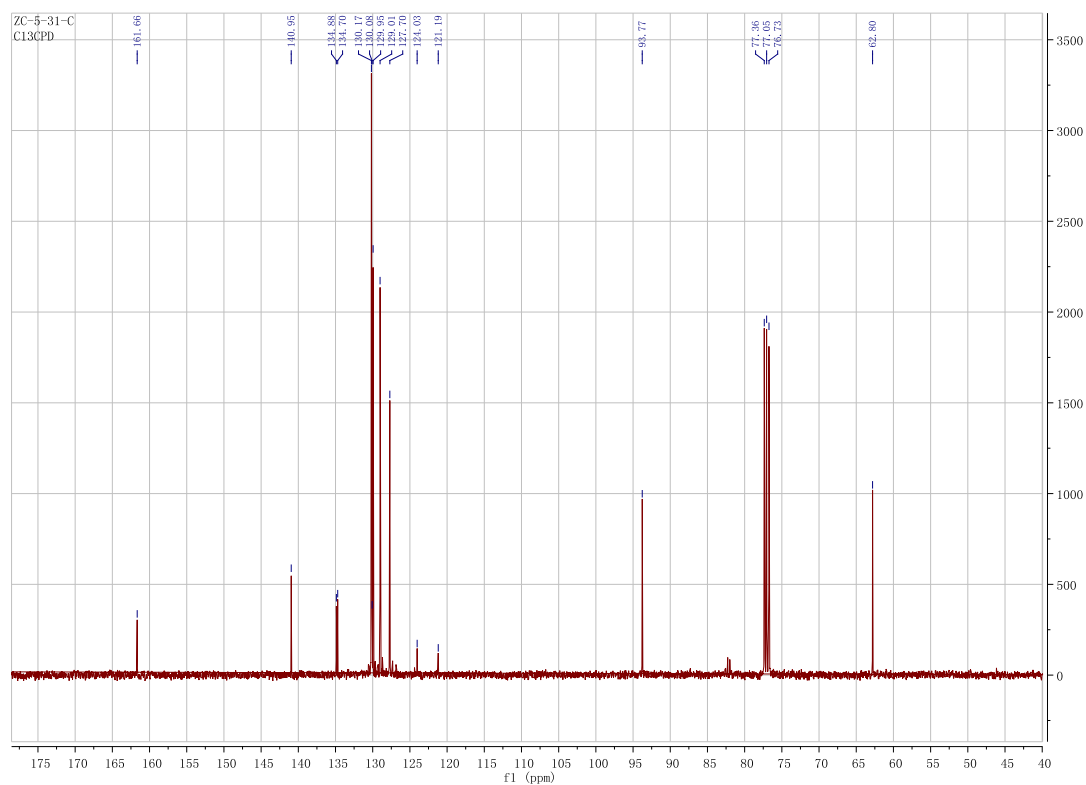
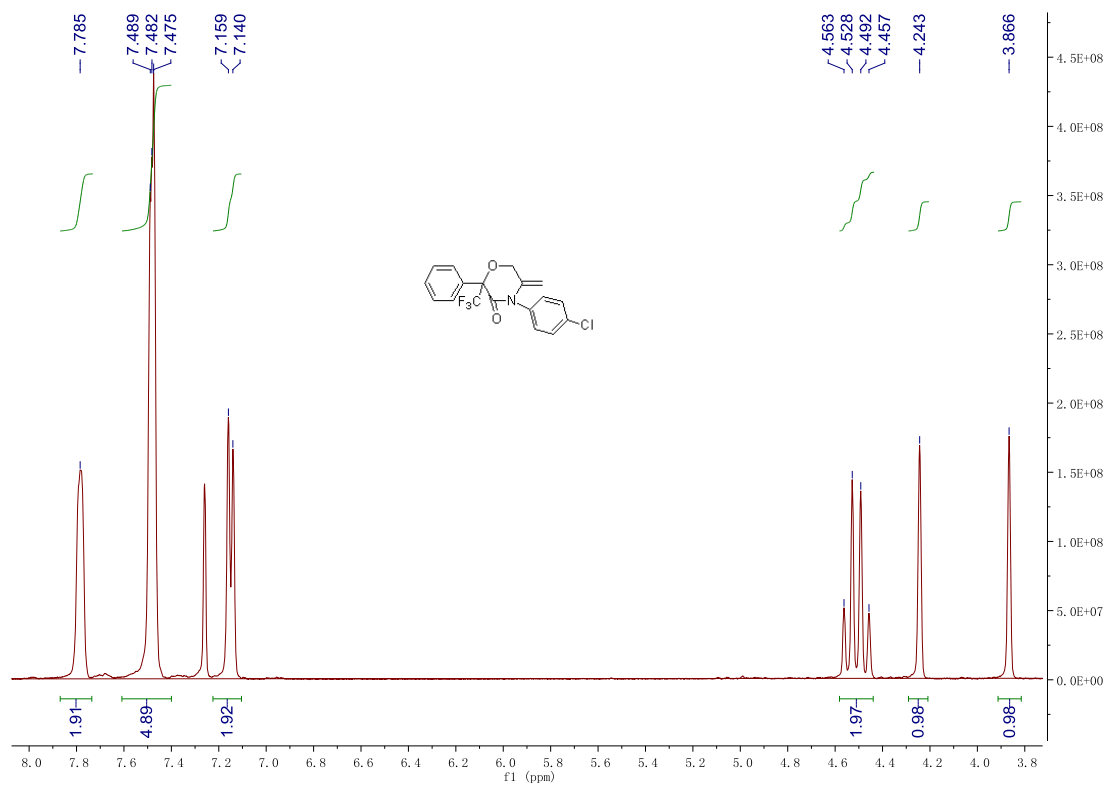
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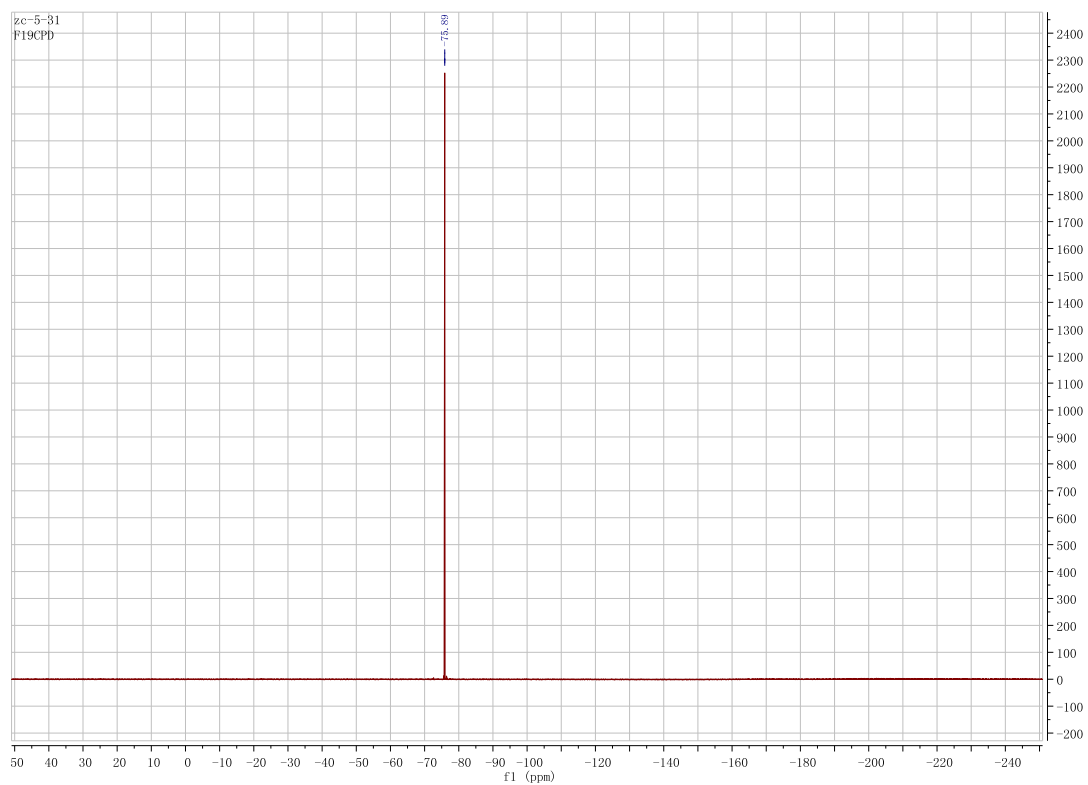
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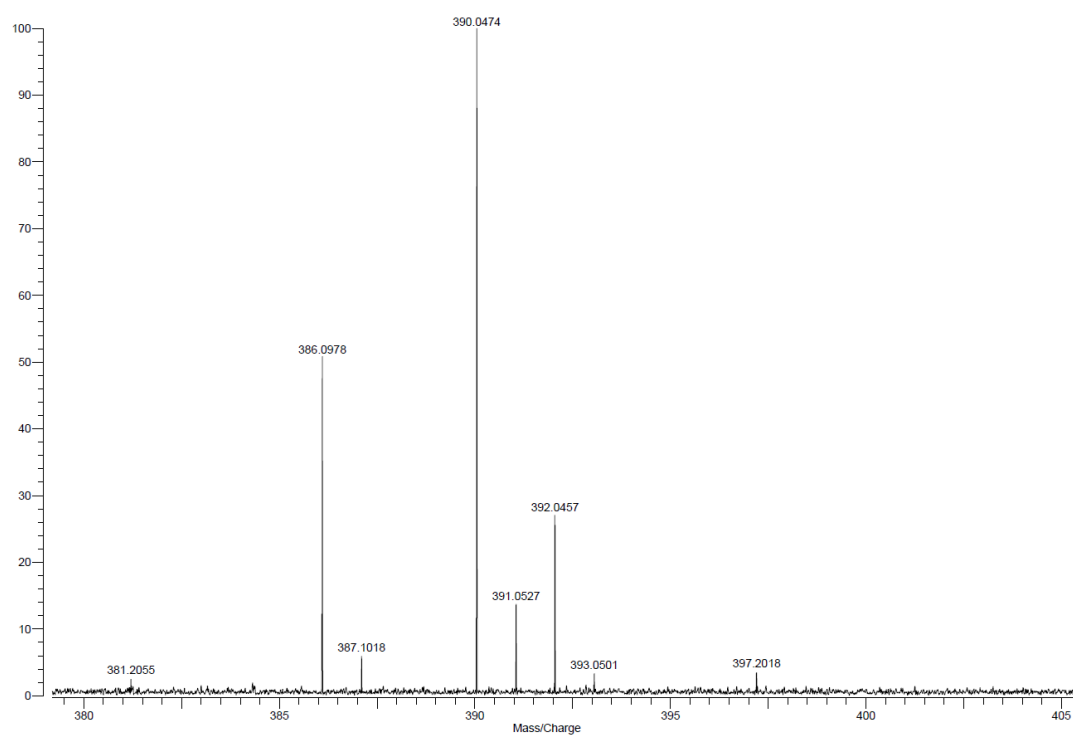
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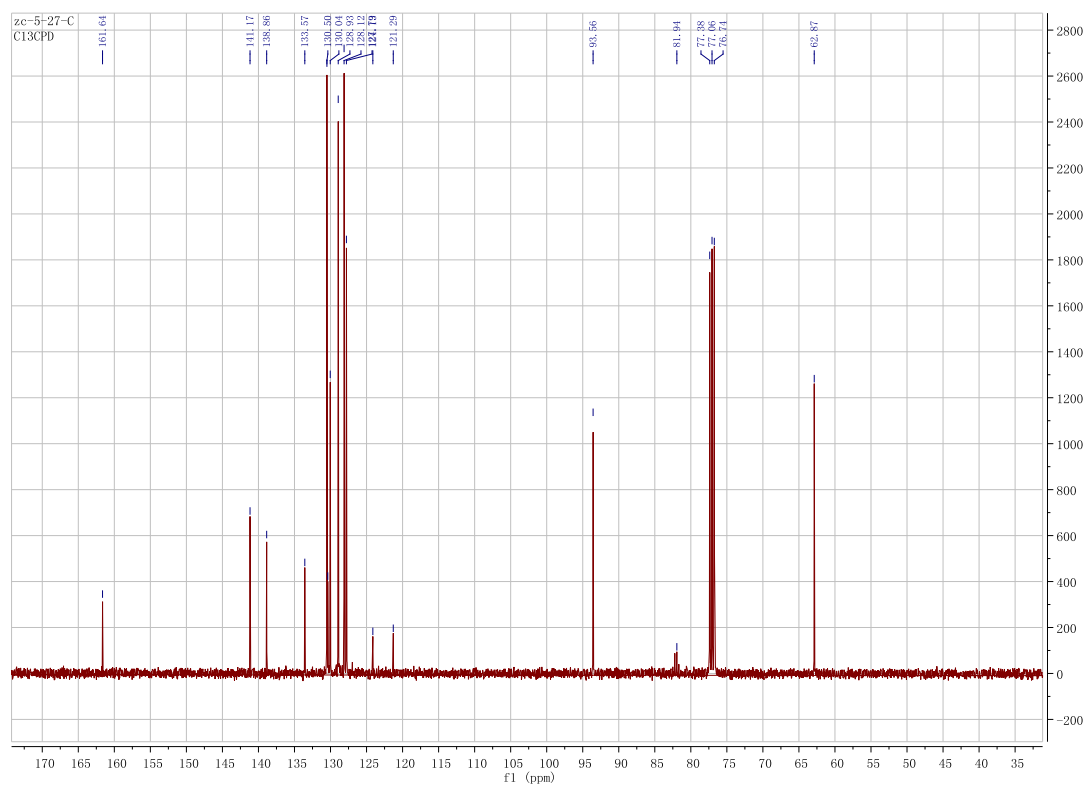
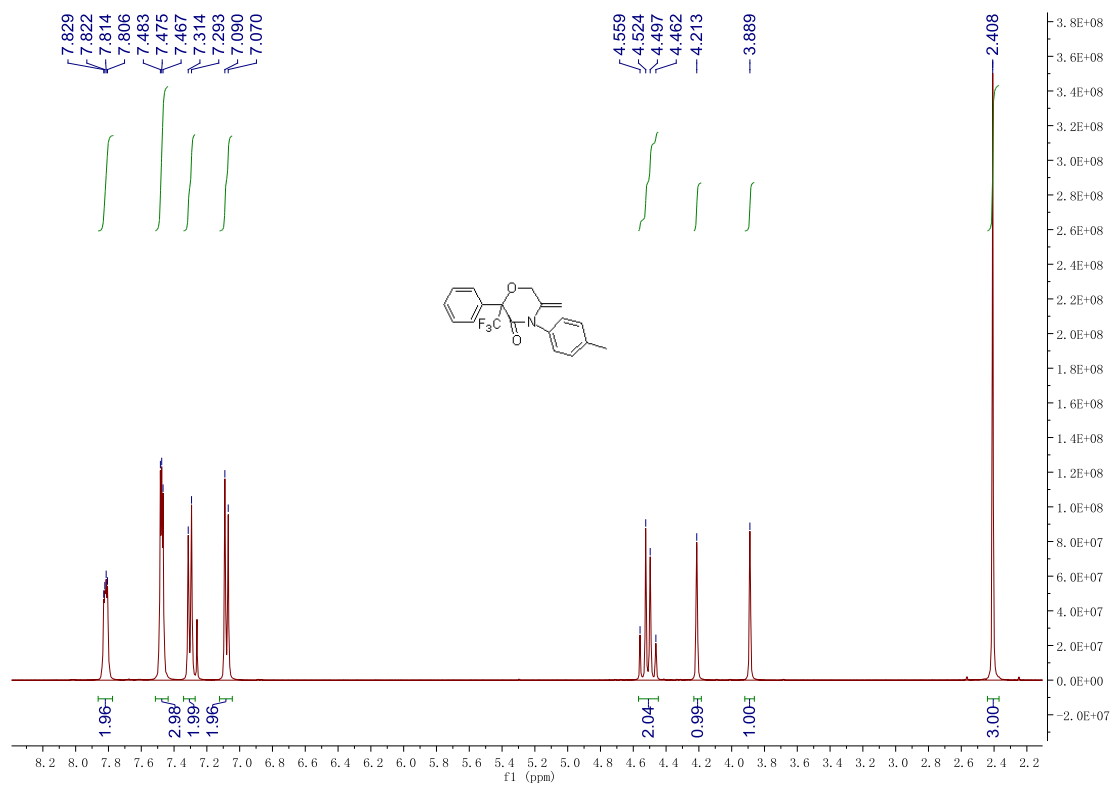


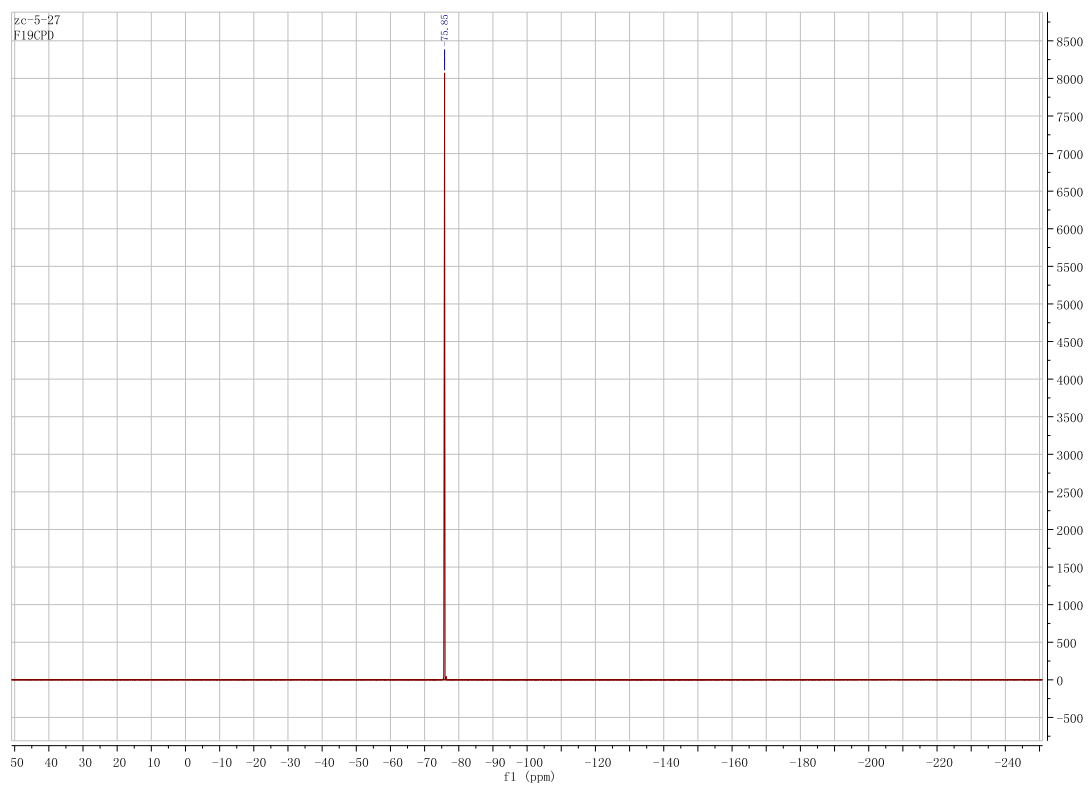
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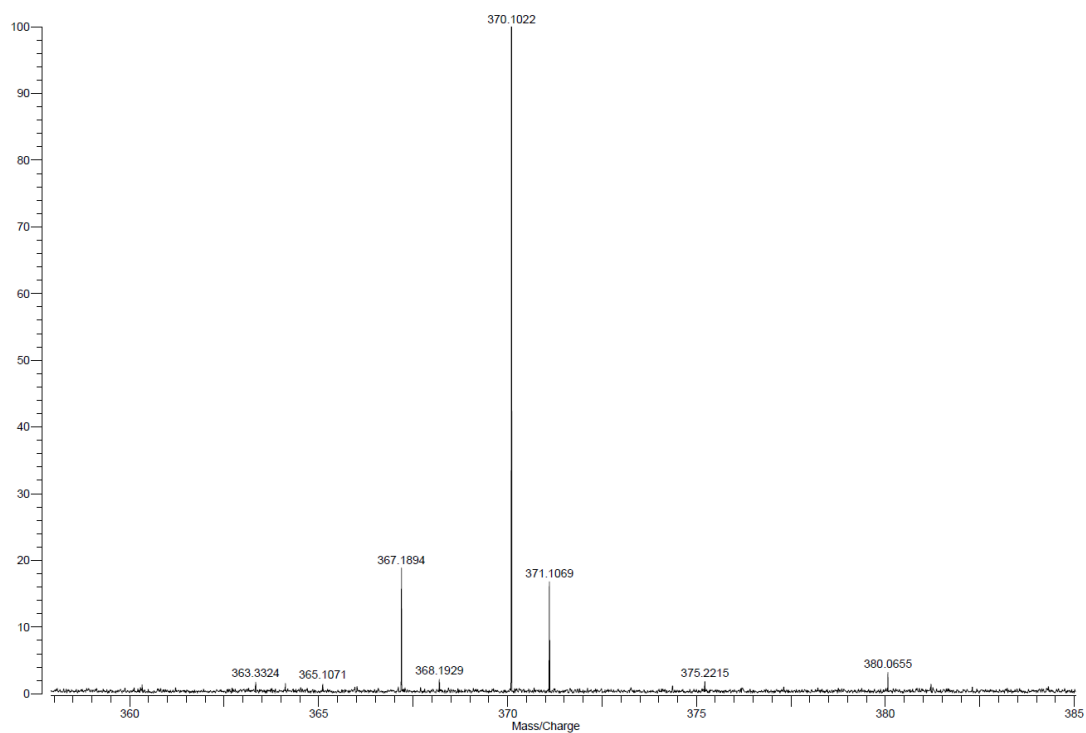
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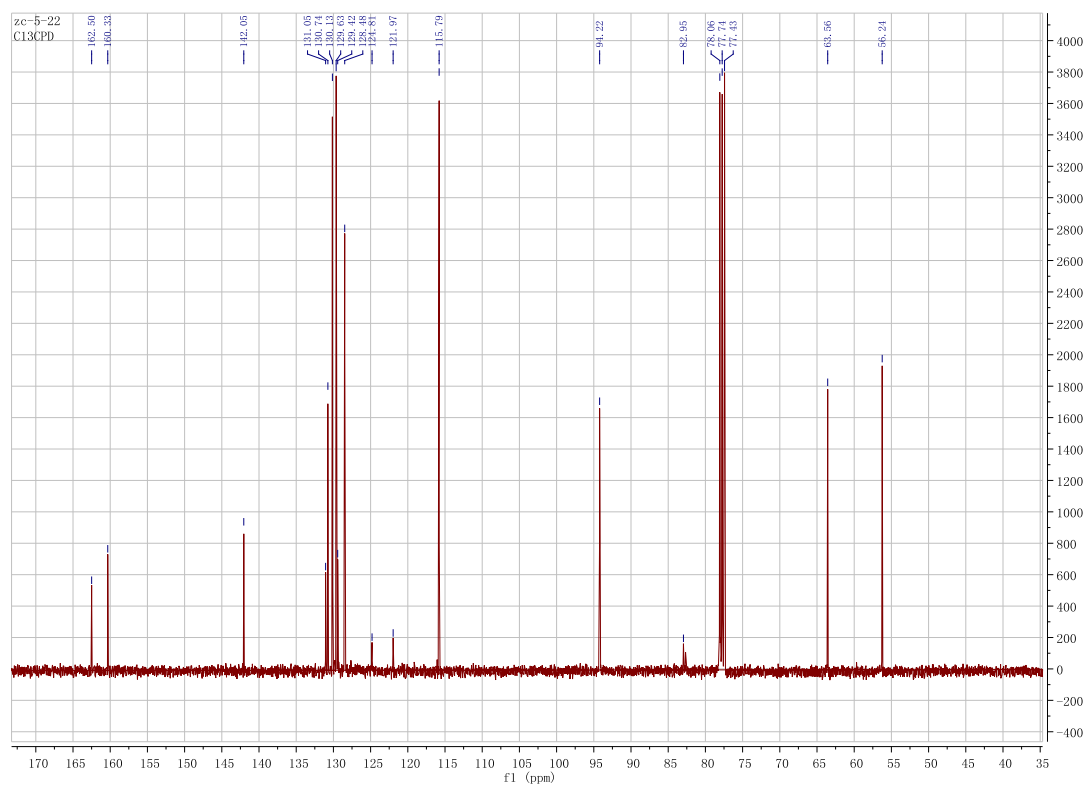
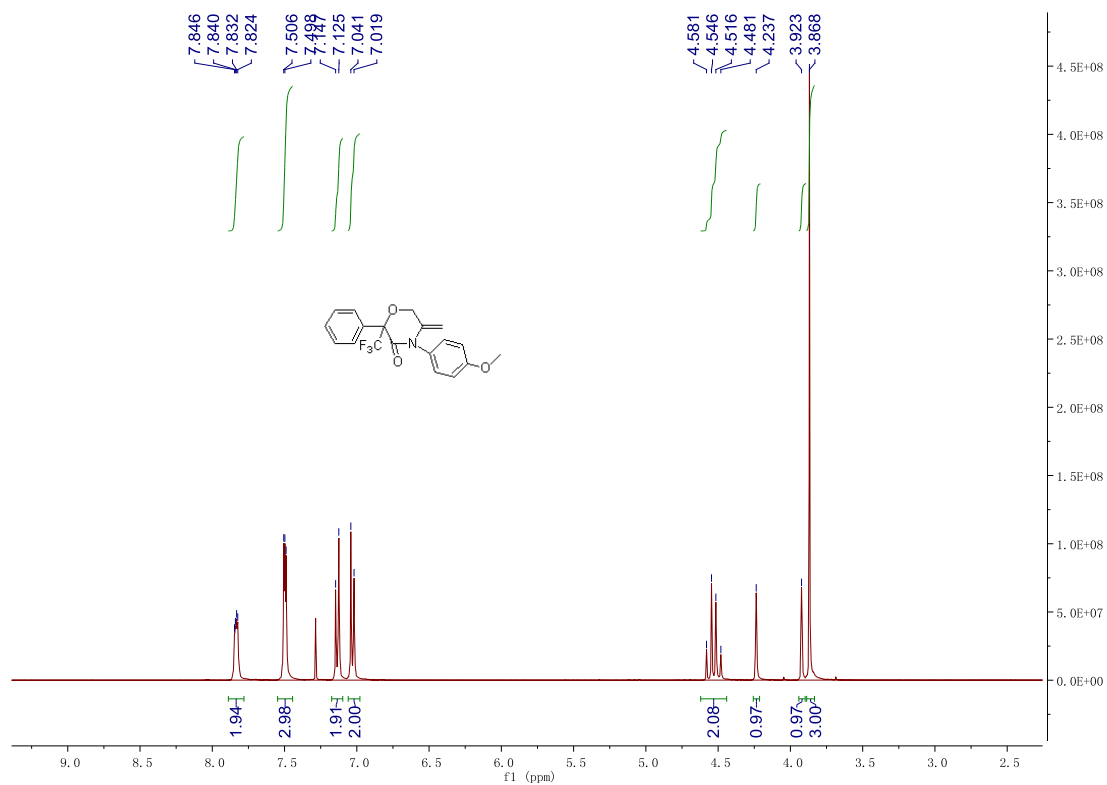


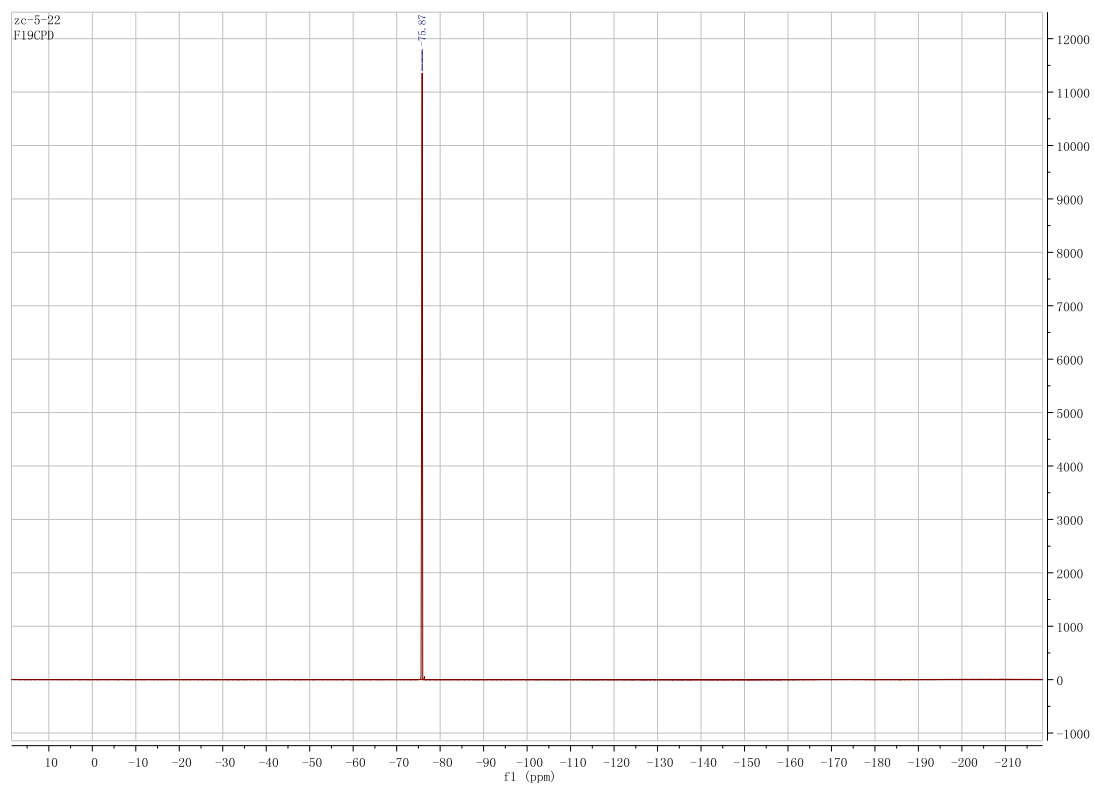
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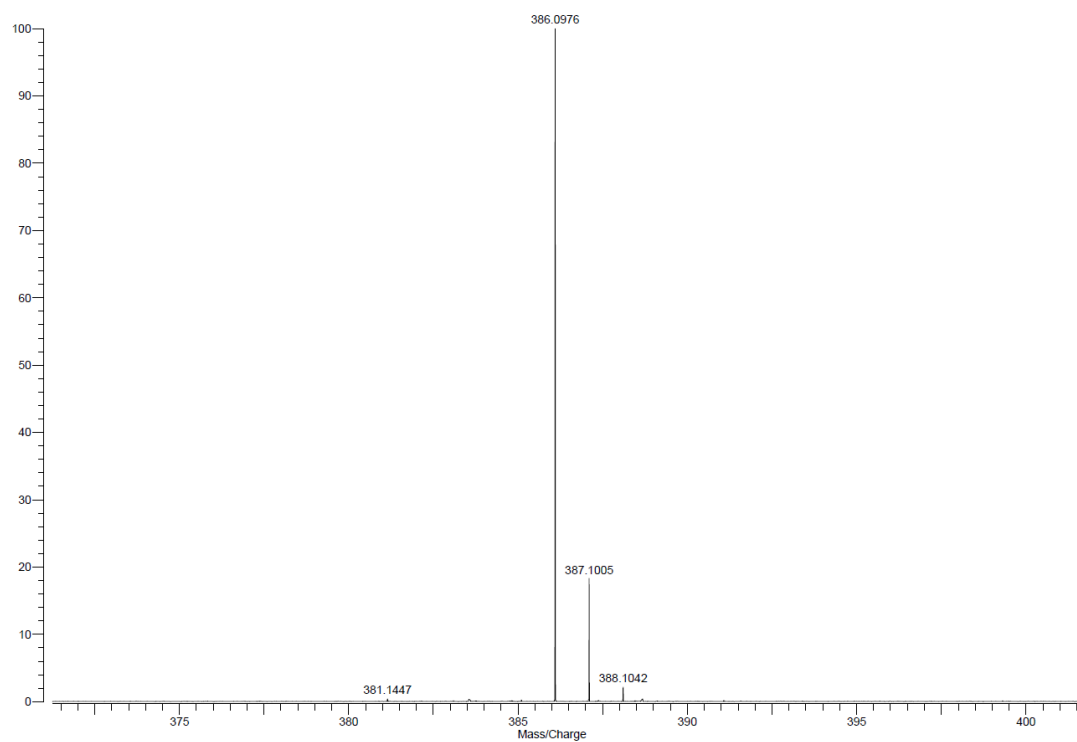




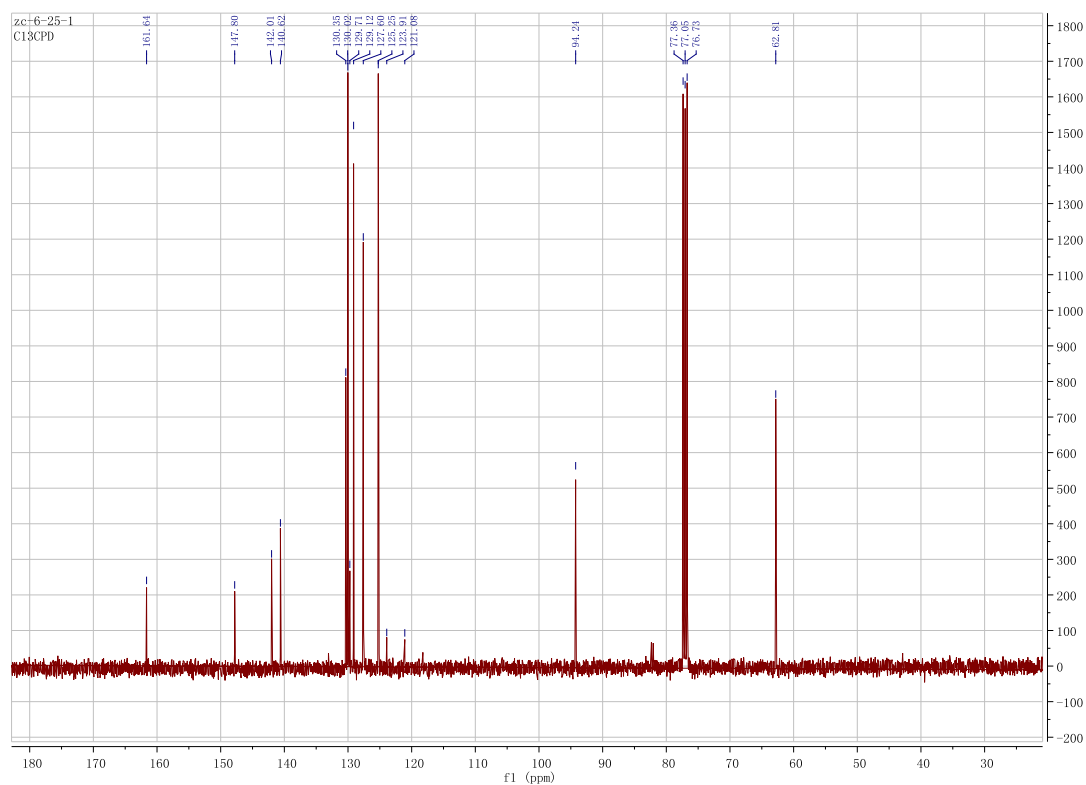
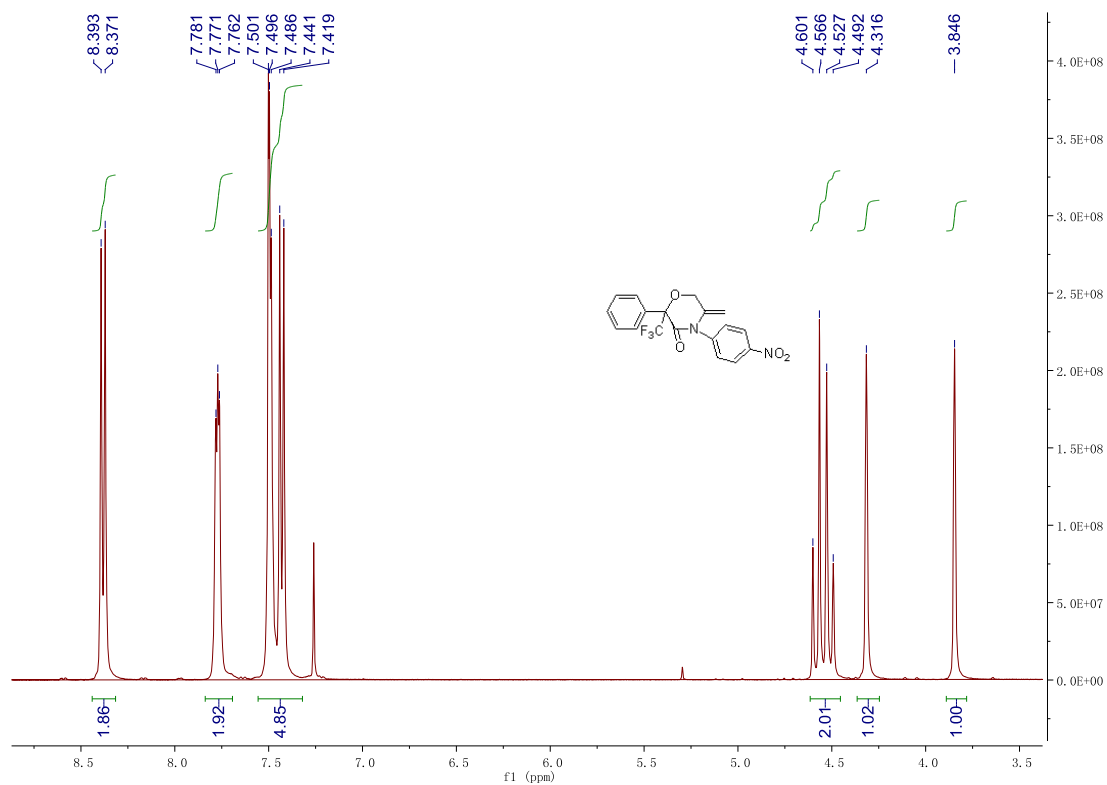
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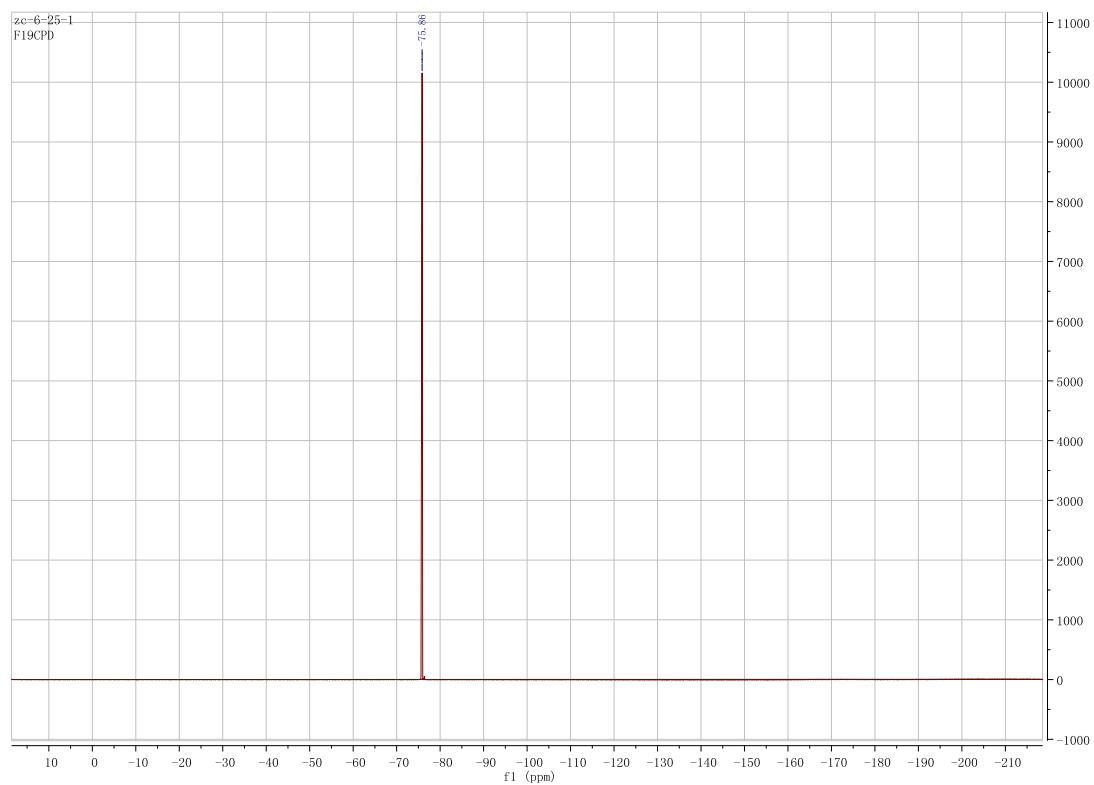
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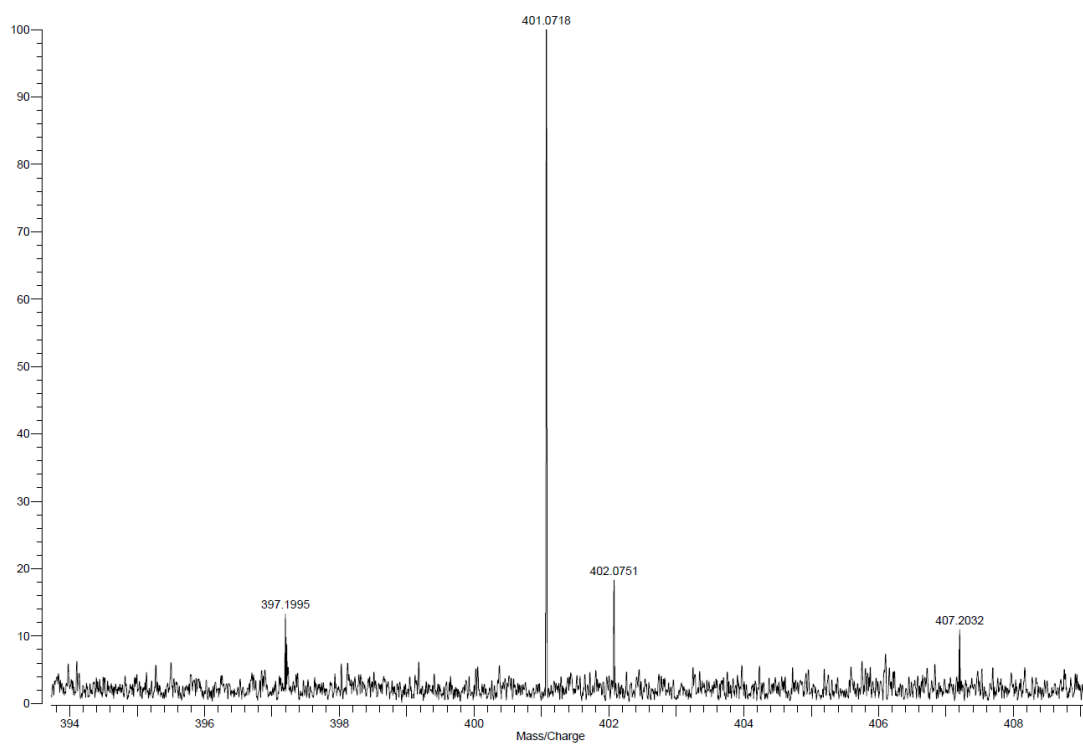




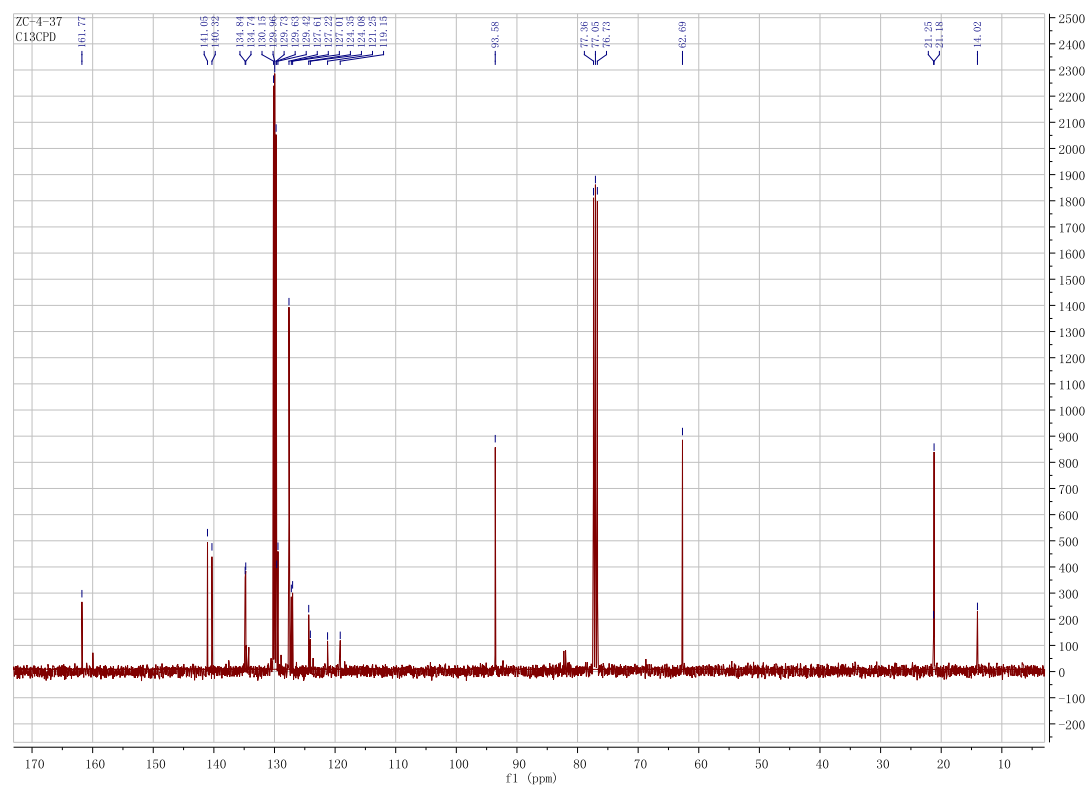
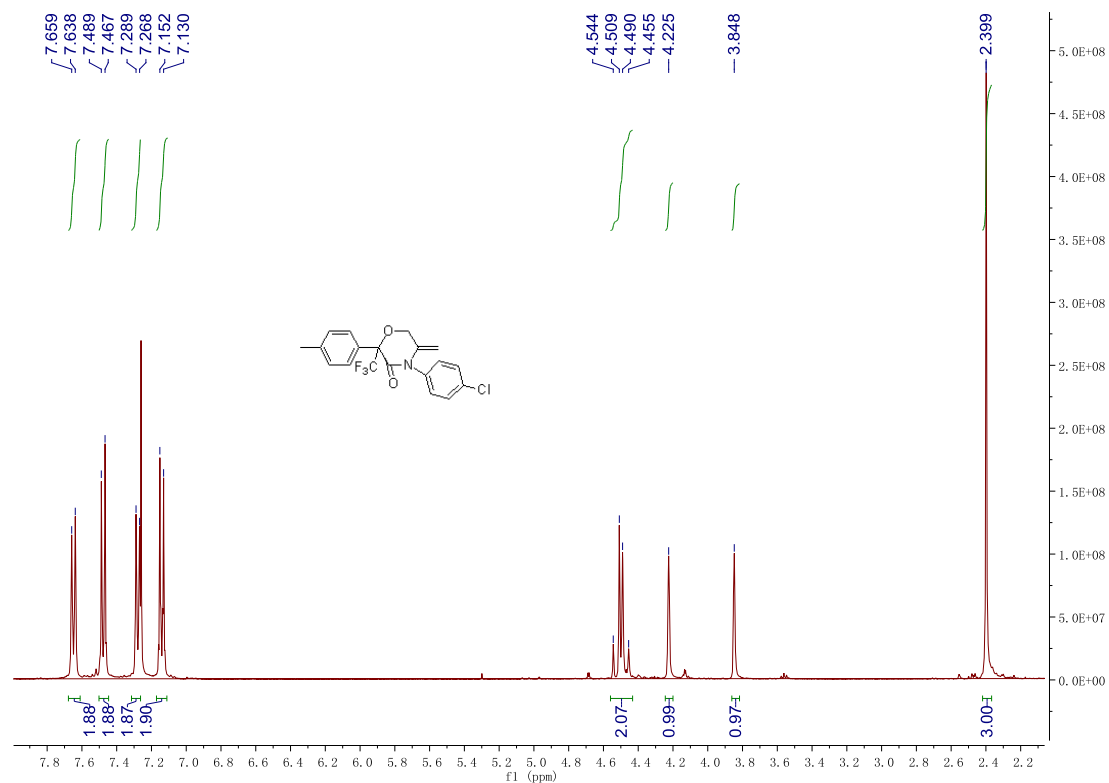
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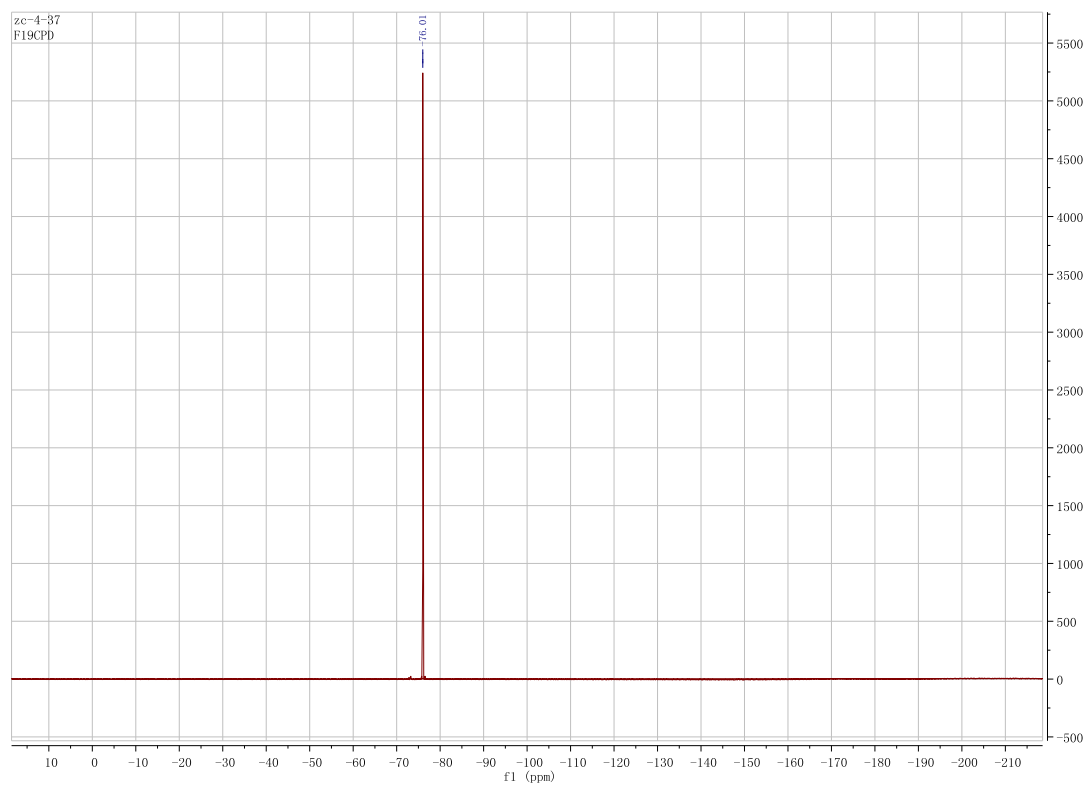
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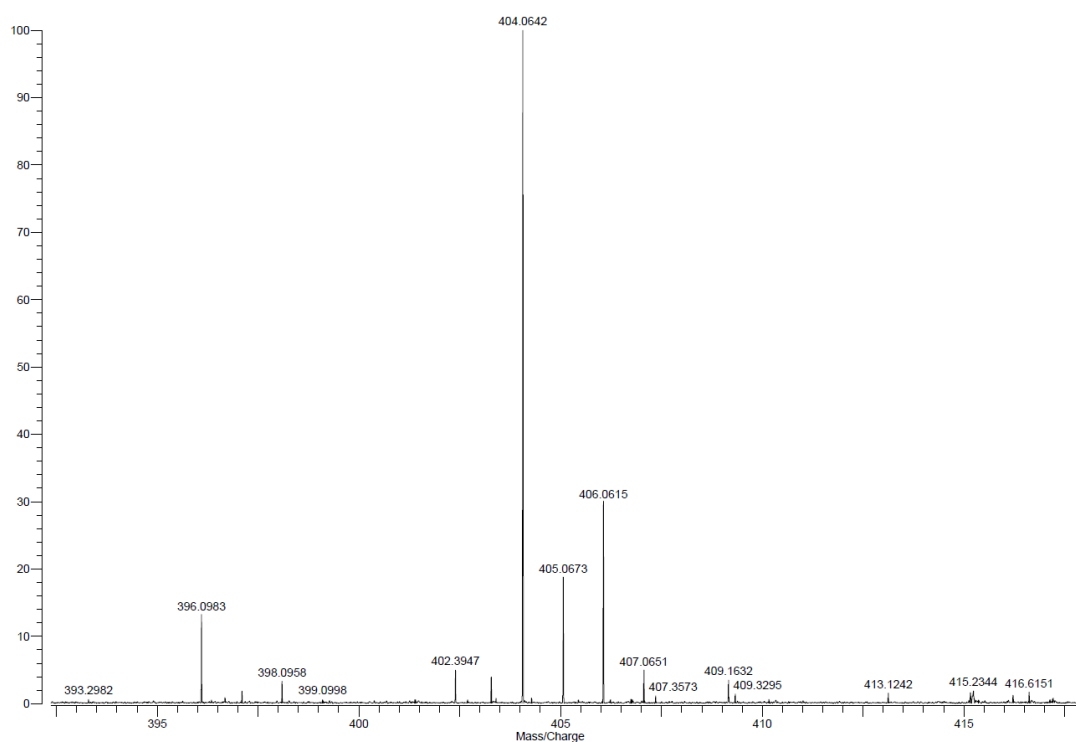




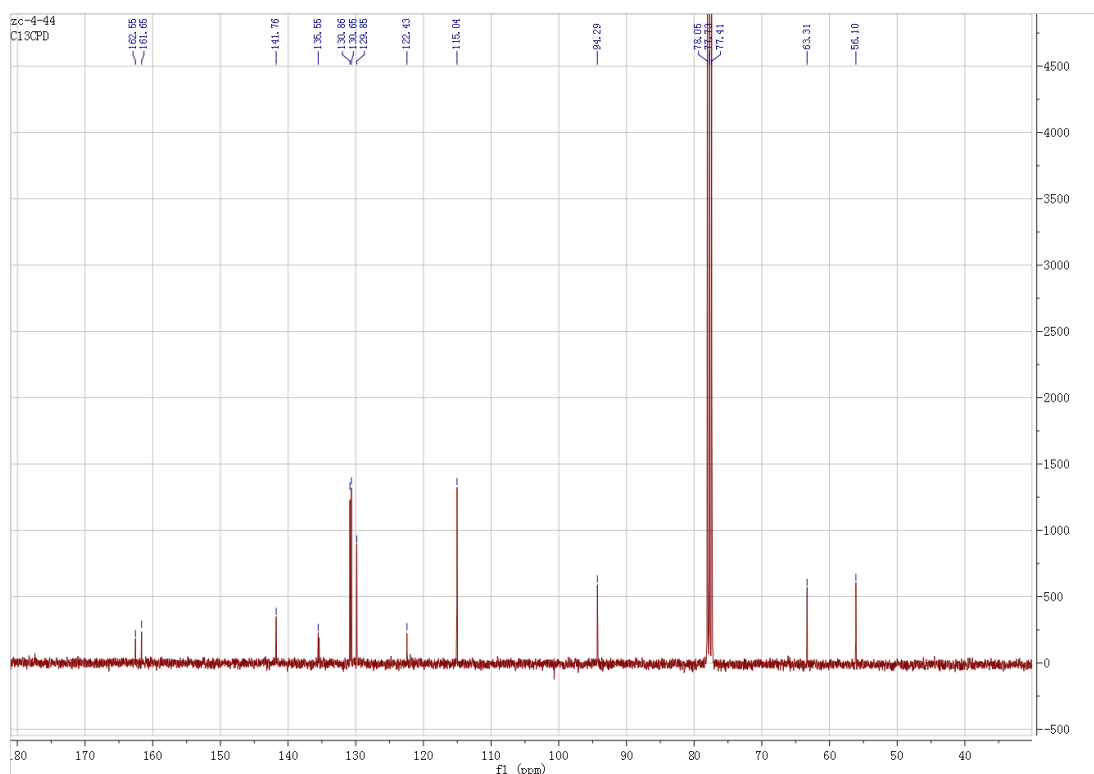
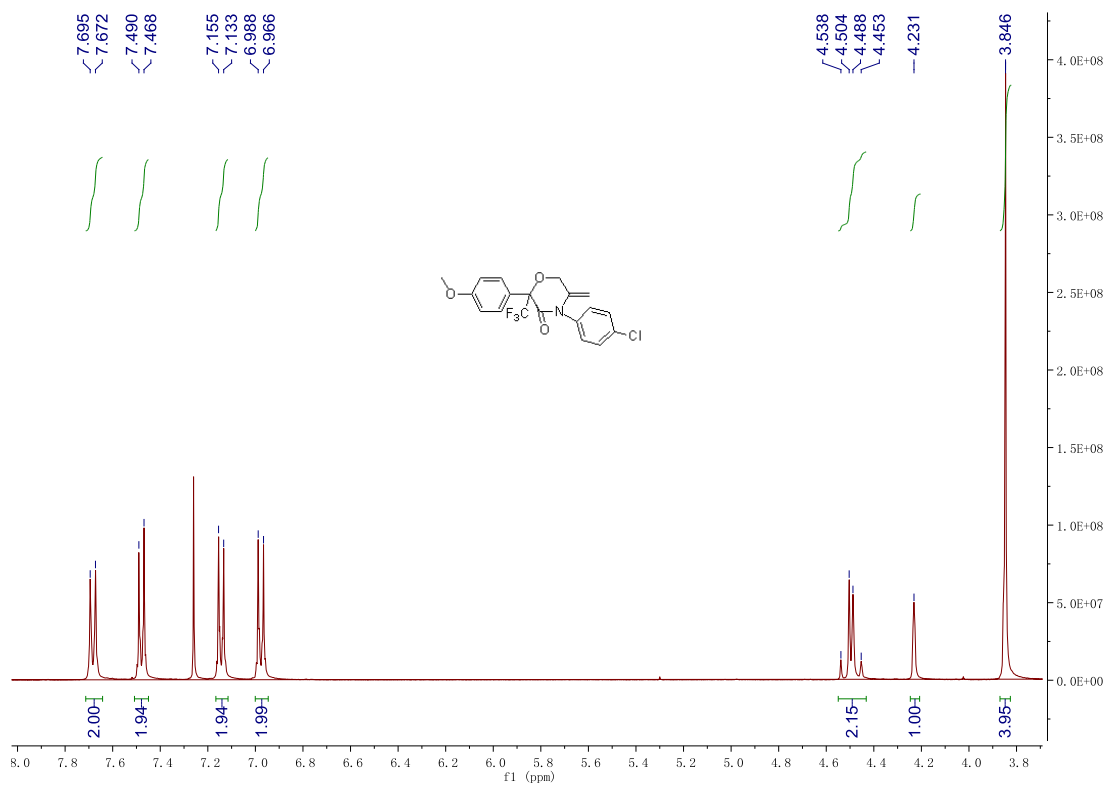
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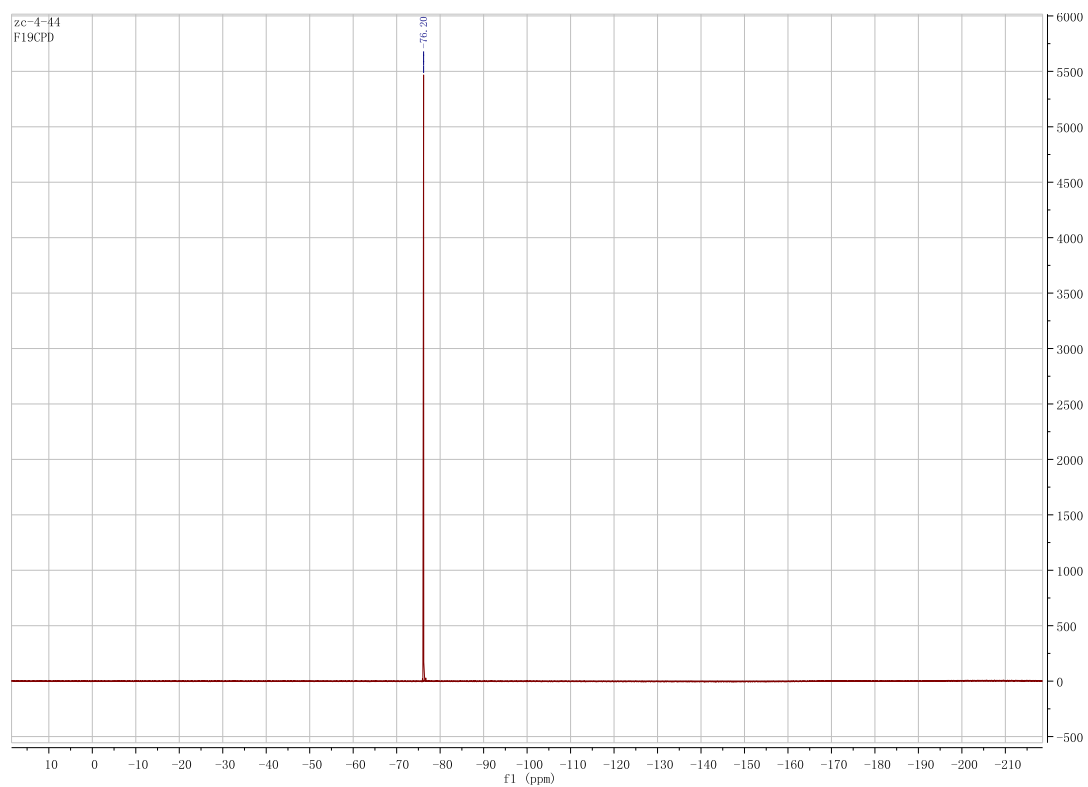
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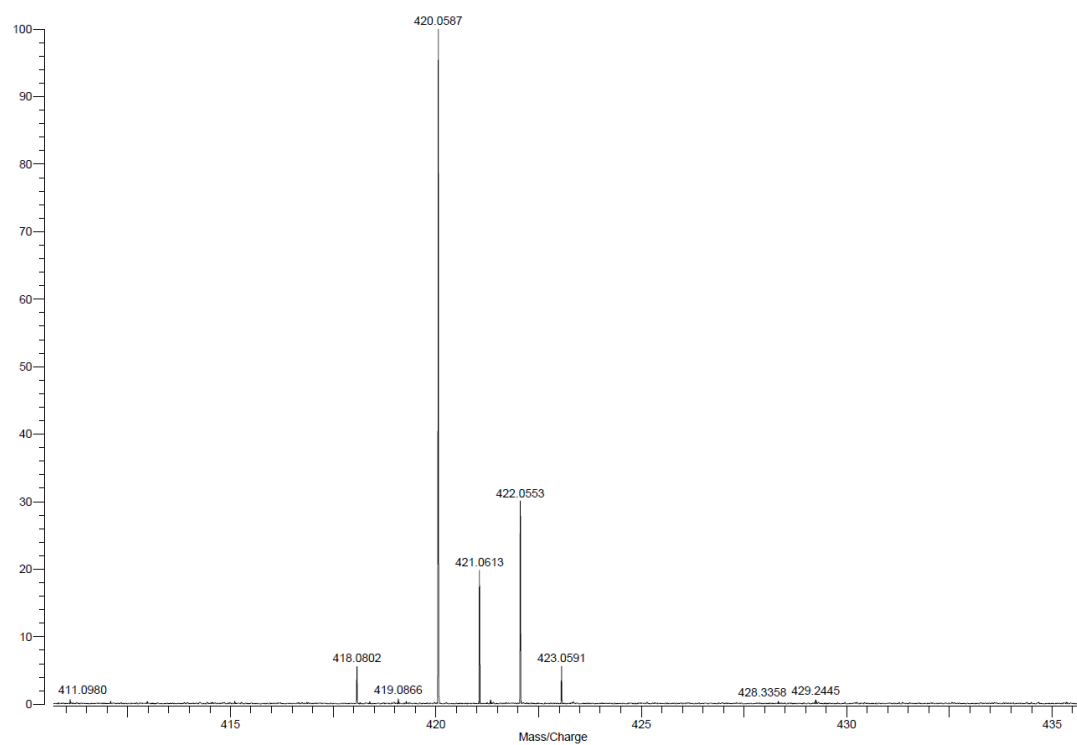




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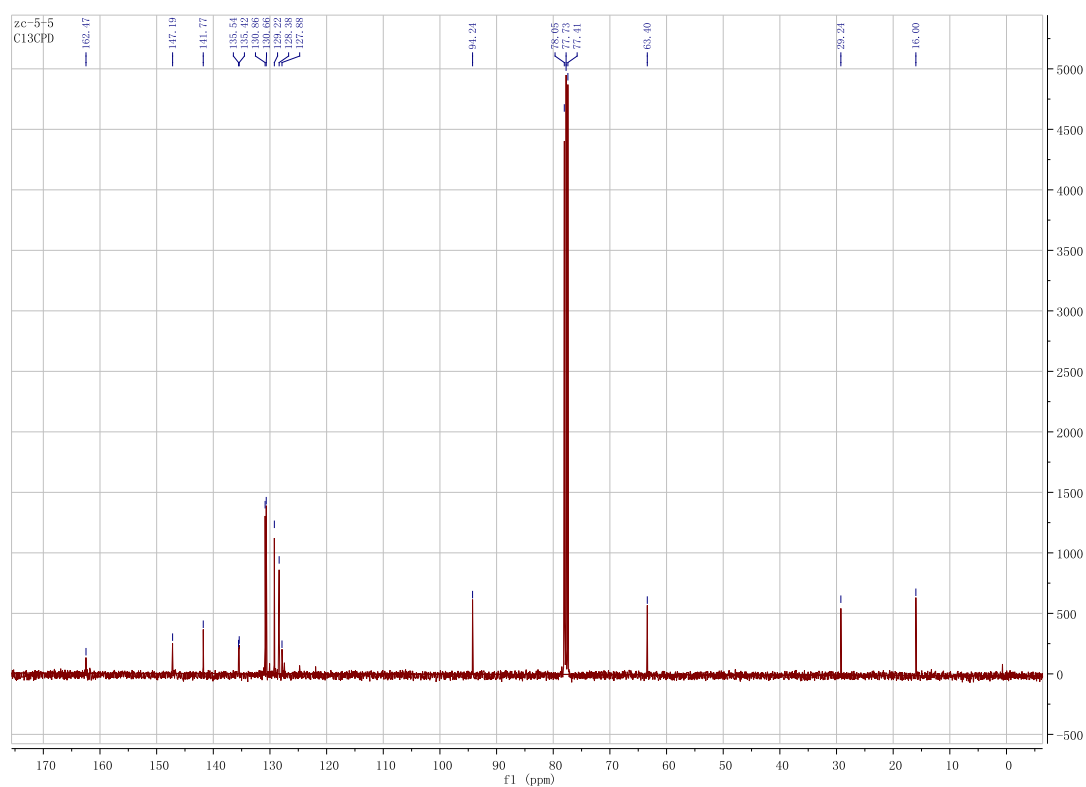
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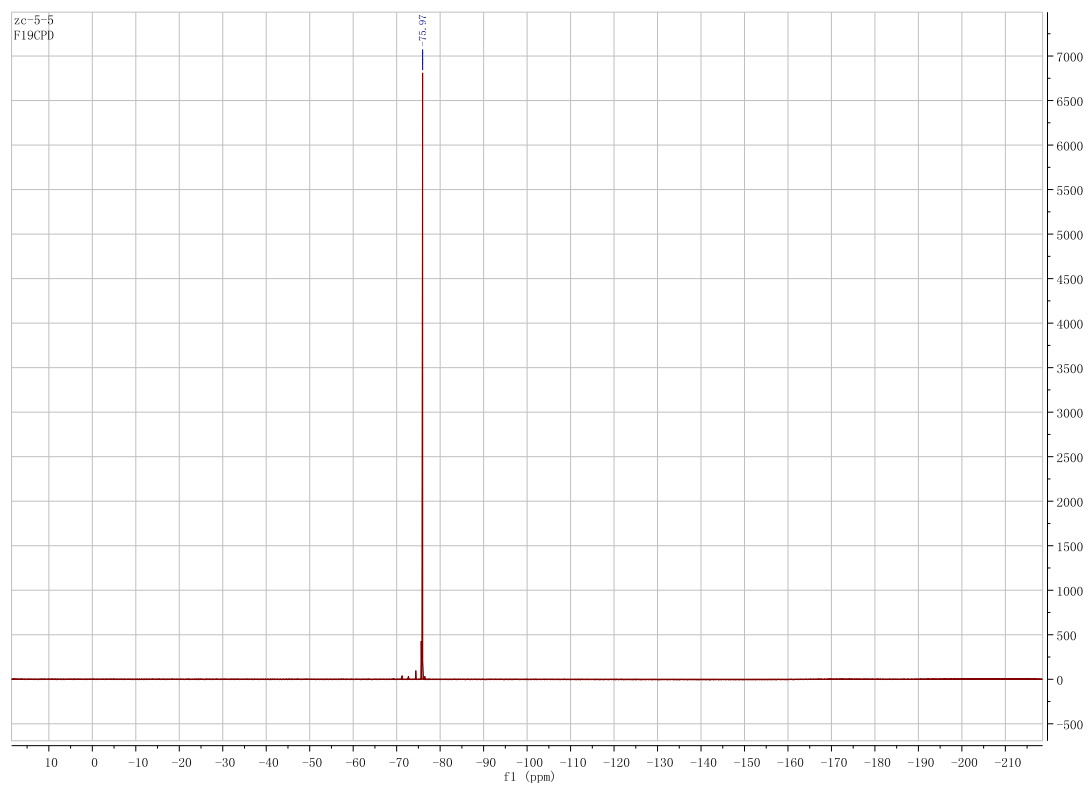
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<sup>1</sup>H NMR spectrum of compound 10 in CDCl<sub>3</sub>. The spectrum shows peaks in the aromatic region (7.1-7.7 ppm) and aliphatic region (2.6-4.5 ppm). Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
7.685	1.74
7.665	1.72
7.491	1.94
7.469	1.76
7.311	
7.290	
7.260	
7.157	
7.136	
4.512	0.89
4.500	0.86
4.226	0.88
3.849	0.87
2.728	2.00
2.709	
2.690	
2.671	

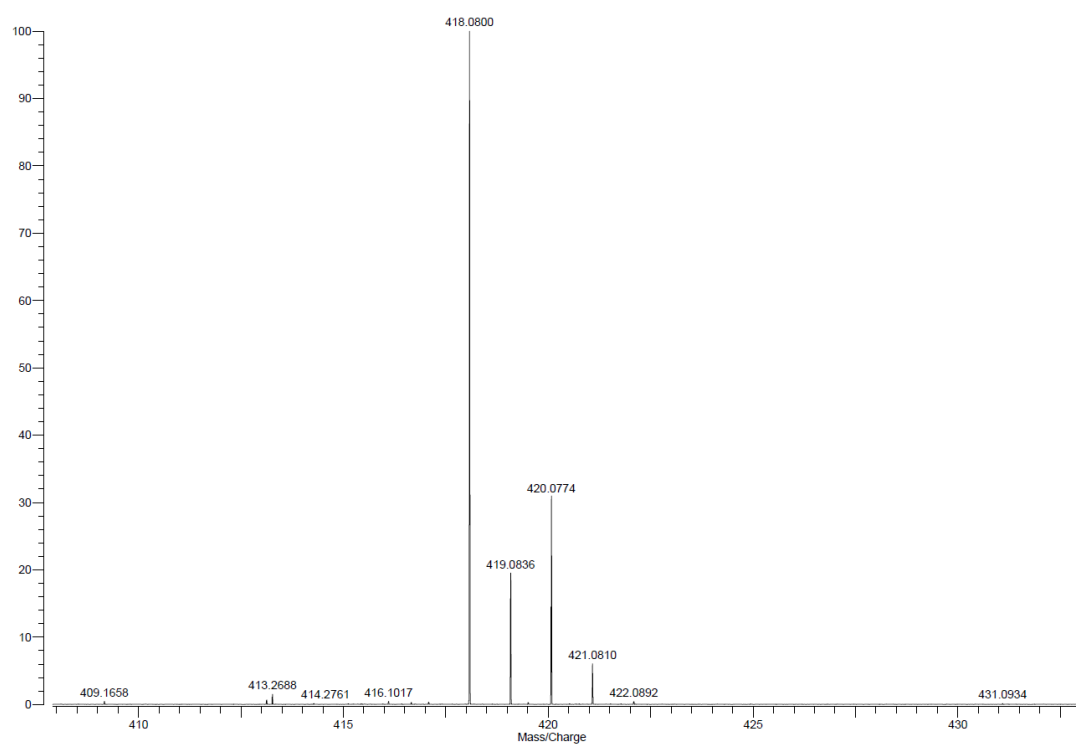




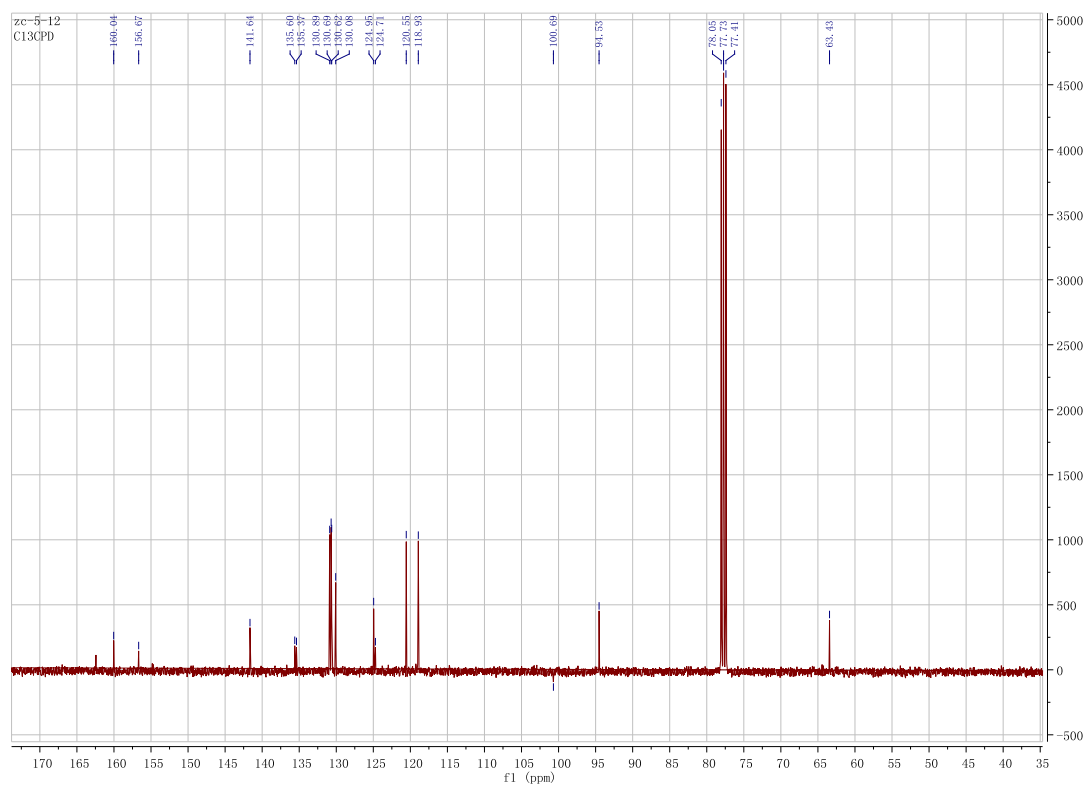
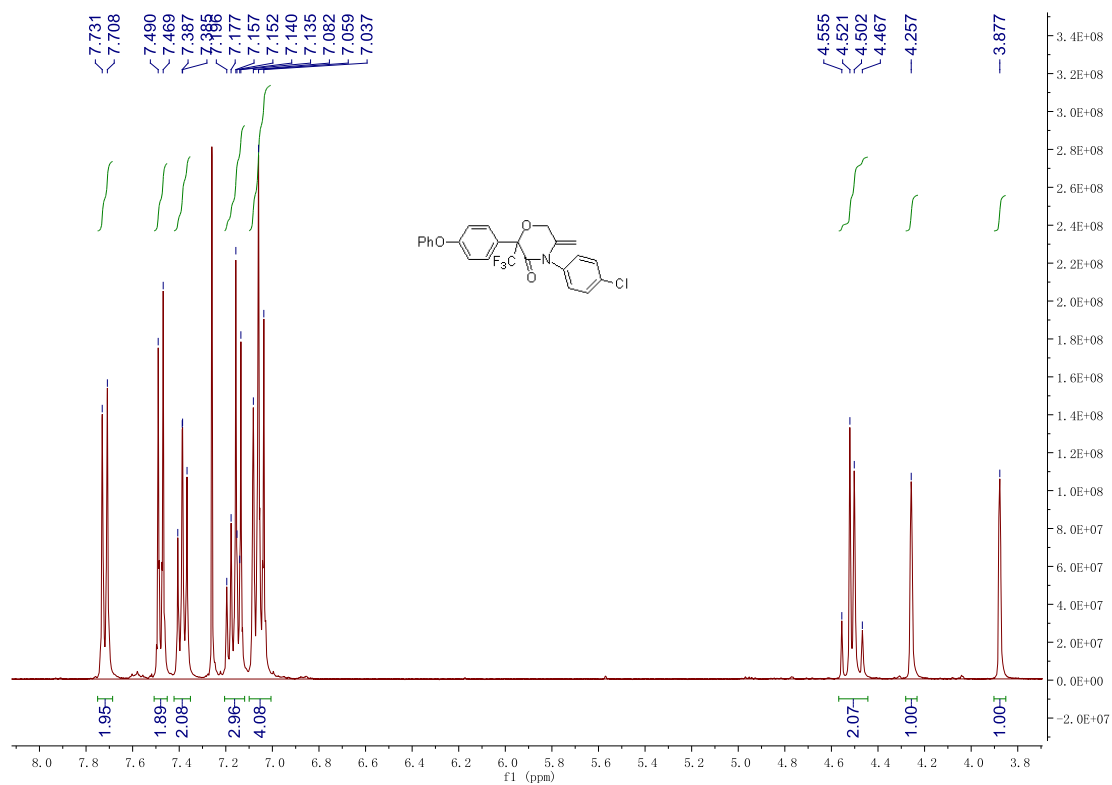
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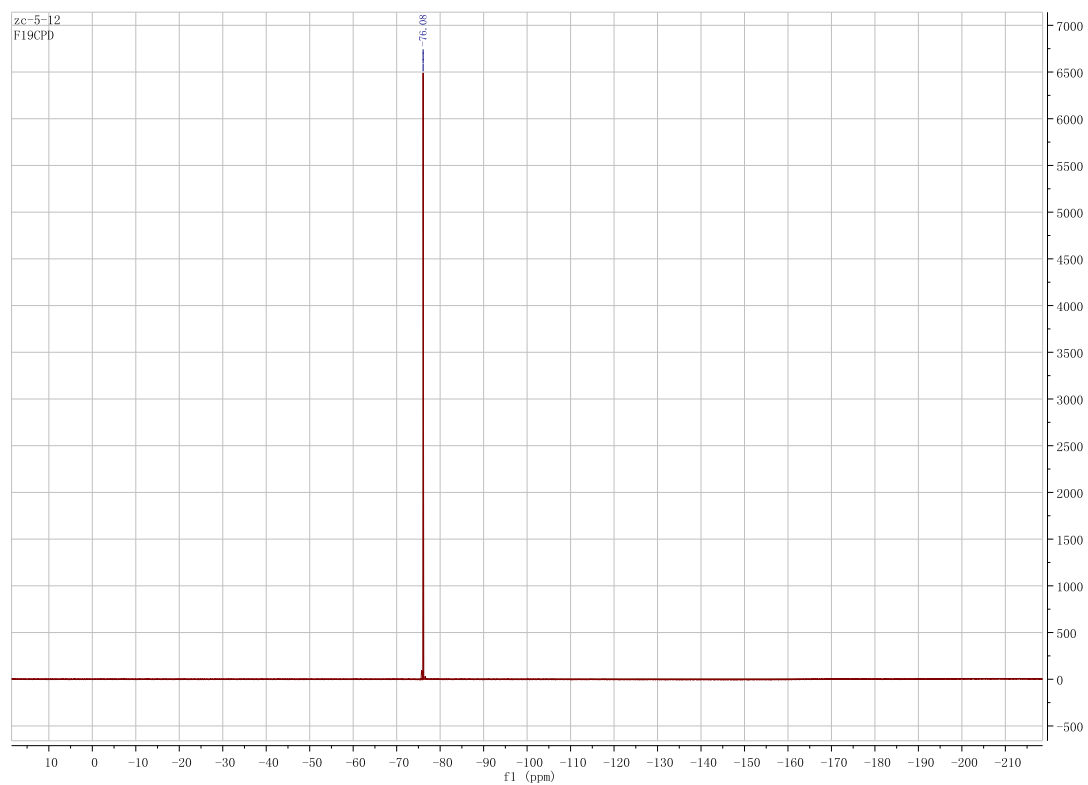
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3k



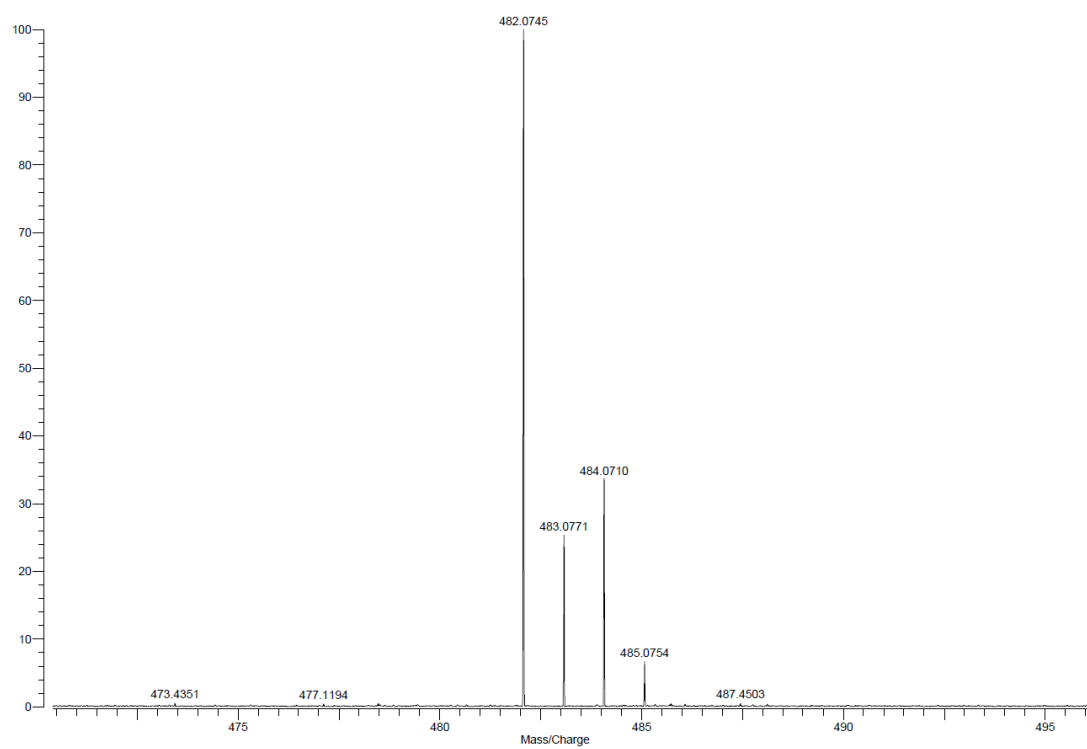




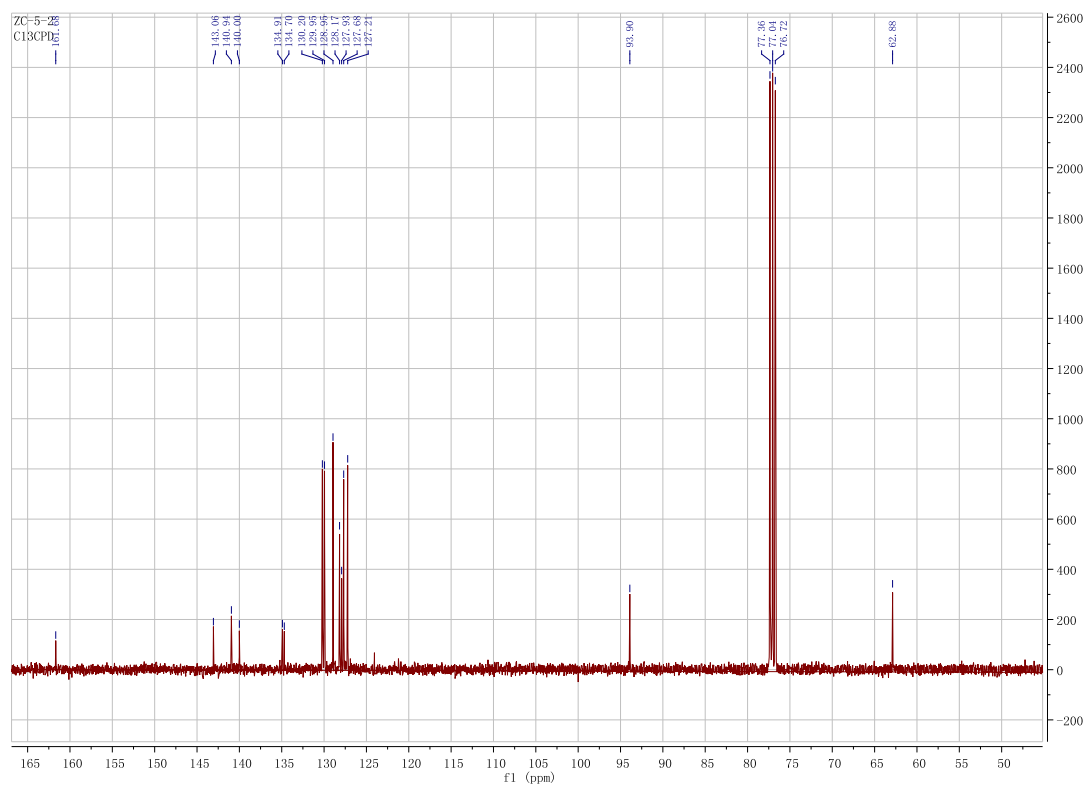
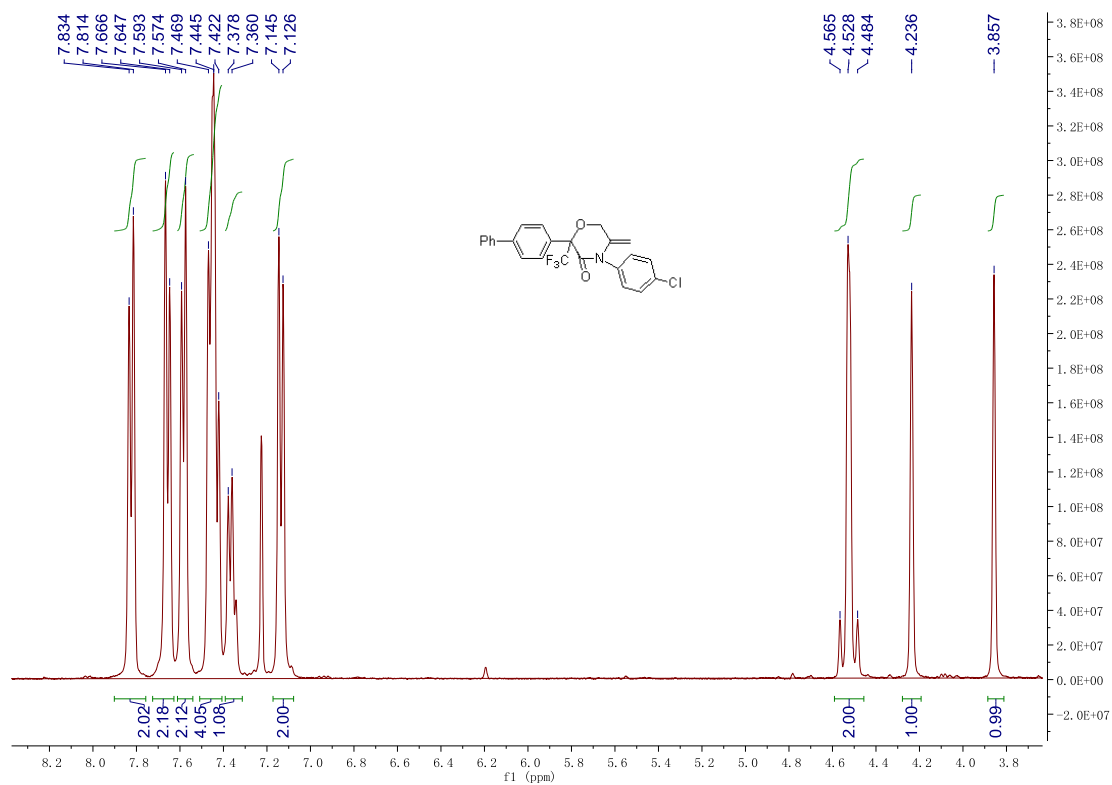
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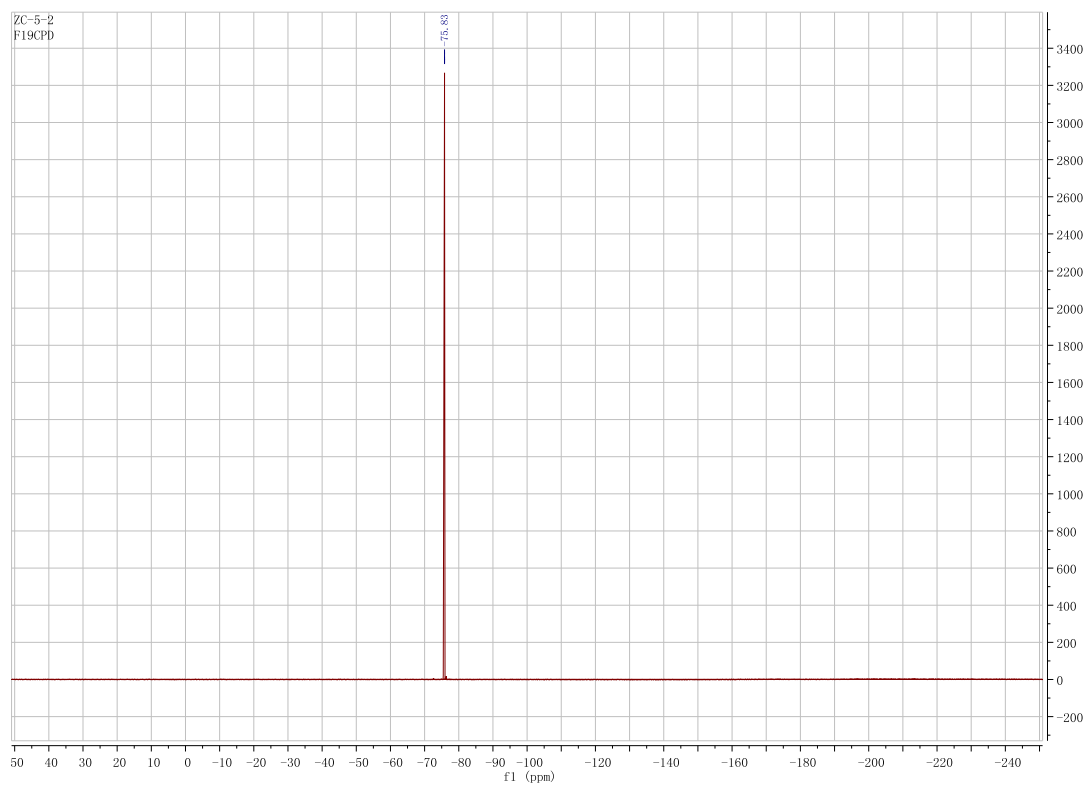
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31

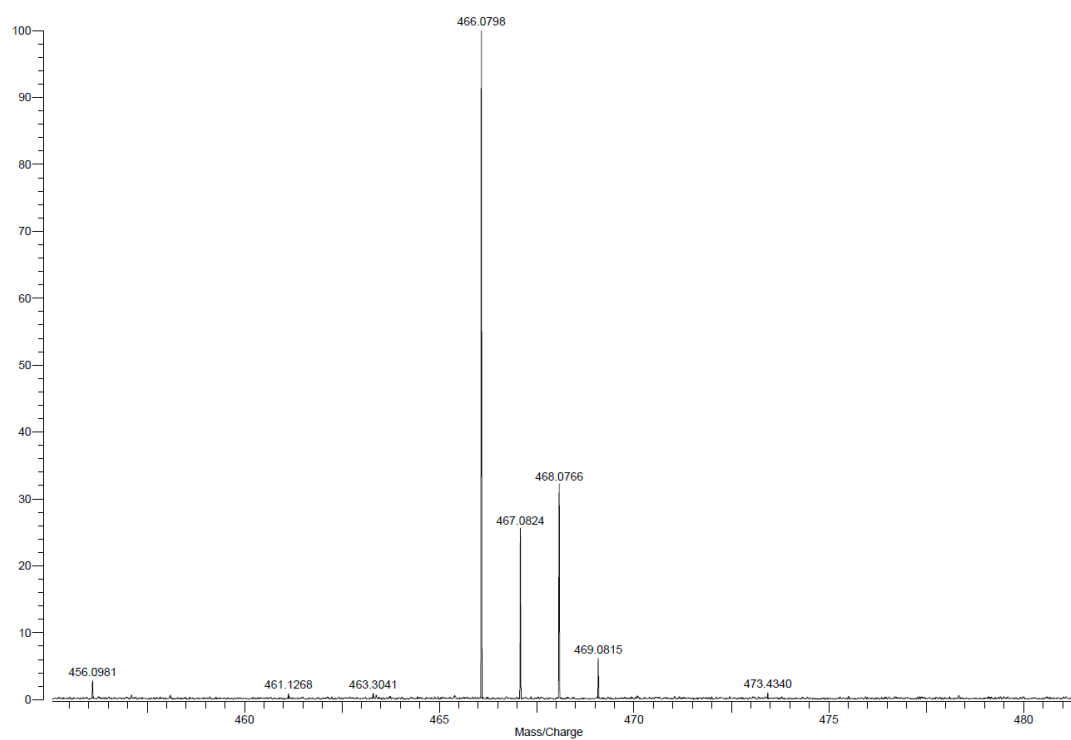


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Varian QFT-ESI  
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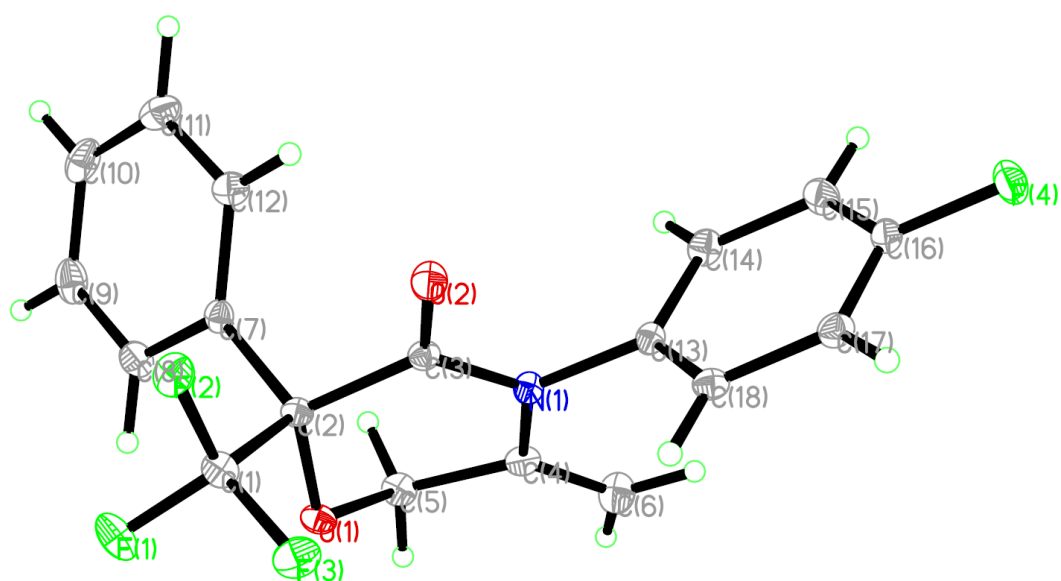


Table 1. Crystal data and structure refinement for 3a.

Identification code	m130413e1
Empirical formula	C <sub>18</sub> H <sub>13</sub> F <sub>4</sub> N O <sub>2</sub>
Formula weight	351.29
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.353(7) Å    alpha = 90 deg. b = 9.575(7) Å    beta = 106.332(8) deg. c = 13.866(7) Å    gamma = 90 deg.
Volume	1573.9(17) Å <sup>3</sup>
Z, Calculated density	4, 1.483 Mg/m <sup>3</sup>
Absorption coefficient	0.129 mm <sup>-1</sup>
F(000)	720
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	1.72 to 27.95 deg.
Limiting indices	-16 ≤ h ≤ 16, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18
Reflections collected / unique	18292 / 3755 [R(int) = 0.0471]
Completeness to theta = 27.95	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9847 and 0.9748
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3755 / 0 / 226
Goodness-of-fit on F <sup>2</sup>	0.993
Final R indices [I > 2σ(I)]	R1 = 0.0360, wR2 = 0.0933
R indices (all data)	R1 = 0.0454, wR2 = 0.0986

Largest diff. peak and hole                      0.255 and -0.289 e.Å<sup>-3</sup>

Table 2. Atomic coordinates ( x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for 3a.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	4440(1)	4300(1)	4035(1)	32(1)
F(2)	3744(1)	3584(1)	5209(1)	27(1)
F(3)	2950(1)	5287(1)	4242(1)	29(1)
F(4)	-3441(1)	3073(1)	3844(1)	31(1)
O(1)	2655(1)	3680(1)	2568(1)	20(1)
O(2)	1507(1)	2821(1)	4570(1)	25(1)
N(1)	633(1)	3075(1)	2904(1)	18(1)
C(1)	3477(1)	4052(1)	4263(1)	22(1)
C(2)	2733(1)	3021(1)	3505(1)	18(1)
C(3)	1573(1)	2955(1)	3712(1)	18(1)
C(4)	669(1)	3179(1)	1887(1)	21(1)
C(5)	1828(1)	3003(1)	1765(1)	23(1)
C(6)	-242(1)	3379(2)	1116(1)	31(1)
C(7)	3301(1)	1580(1)	3585(1)	20(1)
C(8)	4120(1)	1362(1)	3084(1)	27(1)
C(9)	4651(1)	77(2)	3134(1)	33(1)
C(10)	4375(1)	-1002(1)	3689(1)	33(1)
C(11)	3575(1)	-795(1)	4192(1)	32(1)
C(12)	3033(1)	491(1)	4145(1)	25(1)
C(13)	-447(1)	3086(1)	3134(1)	19(1)
C(14)	-1159(1)	1944(1)	2878(1)	23(1)
C(15)	-2182(1)	1942(1)	3112(1)	26(1)
C(16)	-2443(1)	3078(1)	3609(1)	22(1)
C(17)	-1745(1)	4219(1)	3885(1)	22(1)
C(18)	-729(1)	4225(1)	3632(1)	21(1)

Table 3. Bond lengths [Å] and angles [deg] for 3a.

F(1)-C(1)	1.3354(14)
F(2)-C(1)	1.3362(15)
F(3)-C(1)	1.3461(16)

F(4)-C(16)	1.3614(14)
O(1)-C(2)	1.4230(14)
O(1)-C(5)	1.4365(15)
O(2)-C(3)	1.2216(15)
N(1)-C(3)	1.3726(15)
N(1)-C(4)	1.4274(16)
N(1)-C(13)	1.4565(15)
C(1)-C(2)	1.5428(17)
C(2)-C(7)	1.5376(18)
C(2)-C(3)	1.5411(17)
C(4)-C(6)	1.3296(18)
C(4)-C(5)	1.4974(18)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9500
C(6)-H(6B)	0.9500
C(7)-C(12)	1.3943(18)
C(7)-C(8)	1.3953(17)
C(8)-C(9)	1.387(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.386(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.3759(19)
C(10)-H(10)	0.9500
C(11)-C(12)	1.3945(19)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.3854(17)
C(13)-C(18)	1.3871(17)
C(14)-C(15)	1.3899(17)
C(14)-H(14)	0.9500
C(15)-C(16)	1.3736(18)
C(15)-H(15)	0.9500
C(16)-C(17)	1.3771(18)
C(17)-C(18)	1.3945(17)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(2)-O(1)-C(5)	110.98(9)
C(3)-N(1)-C(4)	123.97(10)
C(3)-N(1)-C(13)	116.03(10)
C(4)-N(1)-C(13)	120.00(9)
F(1)-C(1)-F(2)	107.56(10)
F(1)-C(1)-F(3)	107.18(10)

F(2)-C(1)-F(3)	107.51(9)
F(1)-C(1)-C(2)	110.59(9)
F(2)-C(1)-C(2)	112.96(10)
F(3)-C(1)-C(2)	110.80(10)
O(1)-C(2)-C(7)	112.15(9)
O(1)-C(2)-C(3)	111.13(9)
C(7)-C(2)-C(3)	112.24(9)
O(1)-C(2)-C(1)	102.33(9)
C(7)-C(2)-C(1)	110.66(10)
C(3)-C(2)-C(1)	107.81(9)
O(2)-C(3)-N(1)	122.09(11)
O(2)-C(3)-C(2)	120.41(10)
N(1)-C(3)-C(2)	117.50(10)
C(6)-C(4)-N(1)	123.40(12)
C(6)-C(4)-C(5)	123.04(11)
N(1)-C(4)-C(5)	113.54(10)
O(1)-C(5)-C(4)	110.86(10)
O(1)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5A)	109.5
O(1)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	108.1
C(4)-C(6)-H(6A)	120.0
C(4)-C(6)-H(6B)	120.0
H(6A)-C(6)-H(6B)	120.0
C(12)-C(7)-C(8)	119.01(11)
C(12)-C(7)-C(2)	122.47(11)
C(8)-C(7)-C(2)	118.52(10)
C(9)-C(8)-C(7)	120.40(12)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	120.20(13)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(11)-C(10)-C(9)	119.87(12)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	120.49(12)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(7)-C(12)-C(11)	120.03(12)
C(7)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0

C(14)-C(13)-C(18)	121.17(11)
C(14)-C(13)-N(1)	119.55(10)
C(18)-C(13)-N(1)	119.25(10)
C(13)-C(14)-C(15)	119.68(11)
C(13)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
C(16)-C(15)-C(14)	118.20(11)
C(16)-C(15)-H(15)	120.9
C(14)-C(15)-H(15)	120.9
F(4)-C(16)-C(15)	118.26(10)
F(4)-C(16)-C(17)	118.34(11)
C(15)-C(16)-C(17)	123.40(11)
C(16)-C(17)-C(18)	118.11(11)
C(16)-C(17)-H(17)	120.9
C(18)-C(17)-H(17)	120.9
C(13)-C(18)-C(17)	119.43(11)
C(13)-C(18)-H(18)	120.3
C(17)-C(18)-H(18)	120.3

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 3a.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

	U11	U22	U33	U23	U13	U12
F(1)	27(1)	38(1)	34(1)	-13(1)	13(1)	-13(1)
F(2)	29(1)	32(1)	18(1)	-3(1)	1(1)	-1(1)
F(3)	39(1)	21(1)	28(1)	-6(1)	10(1)	2(1)
F(4)	22(1)	36(1)	38(1)	0(1)	15(1)	-1(1)
O(1)	26(1)	21(1)	16(1)	0(1)	8(1)	-4(1)
O(2)	24(1)	37(1)	17(1)	4(1)	8(1)	3(1)
N(1)	18(1)	21(1)	16(1)	-1(1)	6(1)	2(1)
C(1)	24(1)	22(1)	21(1)	-3(1)	8(1)	-2(1)
C(2)	20(1)	19(1)	15(1)	0(1)	6(1)	-1(1)
C(3)	21(1)	16(1)	18(1)	1(1)	7(1)	1(1)
C(4)	28(1)	18(1)	16(1)	-1(1)	7(1)	0(1)
C(5)	27(1)	26(1)	15(1)	-3(1)	6(1)	-2(1)
C(6)	31(1)	42(1)	20(1)	0(1)	6(1)	4(1)
C(7)	18(1)	19(1)	20(1)	-3(1)	3(1)	0(1)
C(8)	24(1)	25(1)	32(1)	-3(1)	10(1)	-3(1)
C(9)	22(1)	34(1)	41(1)	-10(1)	9(1)	3(1)



C(10)	32(1)	25(1)	35(1)	-7(1)	-2(1)	9(1)
C(11)	40(1)	22(1)	30(1)	3(1)	5(1)	2(1)
C(12)	28(1)	24(1)	24(1)	0(1)	8(1)	-1(1)
C(13)	18(1)	20(1)	18(1)	1(1)	4(1)	3(1)
C(14)	25(1)	19(1)	25(1)	-6(1)	6(1)	2(1)
C(15)	24(1)	22(1)	30(1)	-4(1)	6(1)	-5(1)
C(16)	18(1)	25(1)	23(1)	4(1)	7(1)	3(1)
C(17)	27(1)	18(1)	23(1)	-1(1)	10(1)	3(1)
C(18)	24(1)	16(1)	22(1)	0(1)	7(1)	-1(1)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 3a.

	x	y	z	U(eq)
H(5A)	2007	1995	1761	27
H(5B)	1852	3406	1114	27
H(6A)	-963	3460	1228	37
H(6B)	-171	3440	452	37
H(8)	4315	2099	2705	32
H(9)	5205	-65	2788	39
H(10)	4739	-1882	3721	40
H(11)	3390	-1534	4575	38
H(12)	2481	625	4495	30
H(14)	-949	1167	2545	28
H(15)	-2687	1175	2933	31
H(17)	-1950	4979	4236	26
H(18)	-235	5003	3800	25

Table 6. Torsion angles [deg] for m130413e1.

C(5)-O(1)-C(2)-C(7)	71.52(12)
C(5)-O(1)-C(2)-C(3)	-55.02(12)
C(5)-O(1)-C(2)-C(1)	-169.86(9)
F(1)-C(1)-C(2)-O(1)	-54.28(12)
F(2)-C(1)-C(2)-O(1)	-174.89(9)
F(3)-C(1)-C(2)-O(1)	64.42(11)
F(1)-C(1)-C(2)-C(7)	65.39(12)
F(2)-C(1)-C(2)-C(7)	-55.22(12)
F(3)-C(1)-C(2)-C(7)	-175.92(9)
F(1)-C(1)-C(2)-C(3)	-171.52(9)

F(2)-C(1)-C(2)-C(3)	67.87(12)
F(3)-C(1)-C(2)-C(3)	-52.82(12)
C(4)-N(1)-C(3)-O(2)	-177.48(11)
C(13)-N(1)-C(3)-O(2)	2.22(16)
C(4)-N(1)-C(3)-C(2)	3.59(15)
C(13)-N(1)-C(3)-C(2)	-176.71(9)
O(1)-C(2)-C(3)-O(2)	-158.21(10)
C(7)-C(2)-C(3)-O(2)	75.30(13)
C(1)-C(2)-C(3)-O(2)	-46.83(14)
O(1)-C(2)-C(3)-N(1)	20.73(14)
C(7)-C(2)-C(3)-N(1)	-105.75(11)
C(1)-C(2)-C(3)-N(1)	132.12(11)
C(3)-N(1)-C(4)-C(6)	-175.82(12)
C(13)-N(1)-C(4)-C(6)	4.49(17)
C(3)-N(1)-C(4)-C(5)	5.73(15)
C(13)-N(1)-C(4)-C(5)	-173.96(9)
C(2)-O(1)-C(5)-C(4)	65.76(12)
C(6)-C(4)-C(5)-O(1)	142.33(12)
N(1)-C(4)-C(5)-O(1)	-39.22(13)
O(1)-C(2)-C(7)-C(12)	-149.29(11)
C(3)-C(2)-C(7)-C(12)	-23.35(15)
C(1)-C(2)-C(7)-C(12)	97.13(13)
O(1)-C(2)-C(7)-C(8)	31.23(14)
C(3)-C(2)-C(7)-C(8)	157.17(10)
C(1)-C(2)-C(7)-C(8)	-82.34(13)
C(12)-C(7)-C(8)-C(9)	0.64(18)
C(2)-C(7)-C(8)-C(9)	-179.87(11)
C(7)-C(8)-C(9)-C(10)	-0.3(2)
C(8)-C(9)-C(10)-C(11)	-0.1(2)
C(9)-C(10)-C(11)-C(12)	0.3(2)
C(8)-C(7)-C(12)-C(11)	-0.46(18)
C(2)-C(7)-C(12)-C(11)	-179.94(11)
C(10)-C(11)-C(12)-C(7)	-0.01(19)
C(3)-N(1)-C(13)-C(14)	-109.13(12)
C(4)-N(1)-C(13)-C(14)	70.58(14)
C(3)-N(1)-C(13)-C(18)	68.90(14)
C(4)-N(1)-C(13)-C(18)	-111.38(12)
C(18)-C(13)-C(14)-C(15)	0.86(18)
N(1)-C(13)-C(14)-C(15)	178.86(10)
C(13)-C(14)-C(15)-C(16)	-1.08(18)
C(14)-C(15)-C(16)-F(4)	-179.63(10)
C(14)-C(15)-C(16)-C(17)	0.20(19)
F(4)-C(16)-C(17)-C(18)	-179.27(10)

C(15)-C(16)-C(17)-C(18)	0.91(18)
C(14)-C(13)-C(18)-C(17)	0.26(17)
N(1)-C(13)-C(18)-C(17)	-177.75(10)
C(16)-C(17)-C(18)-C(13)	-1.12(16)

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Symmetry transformations used to generate equivalent atoms:

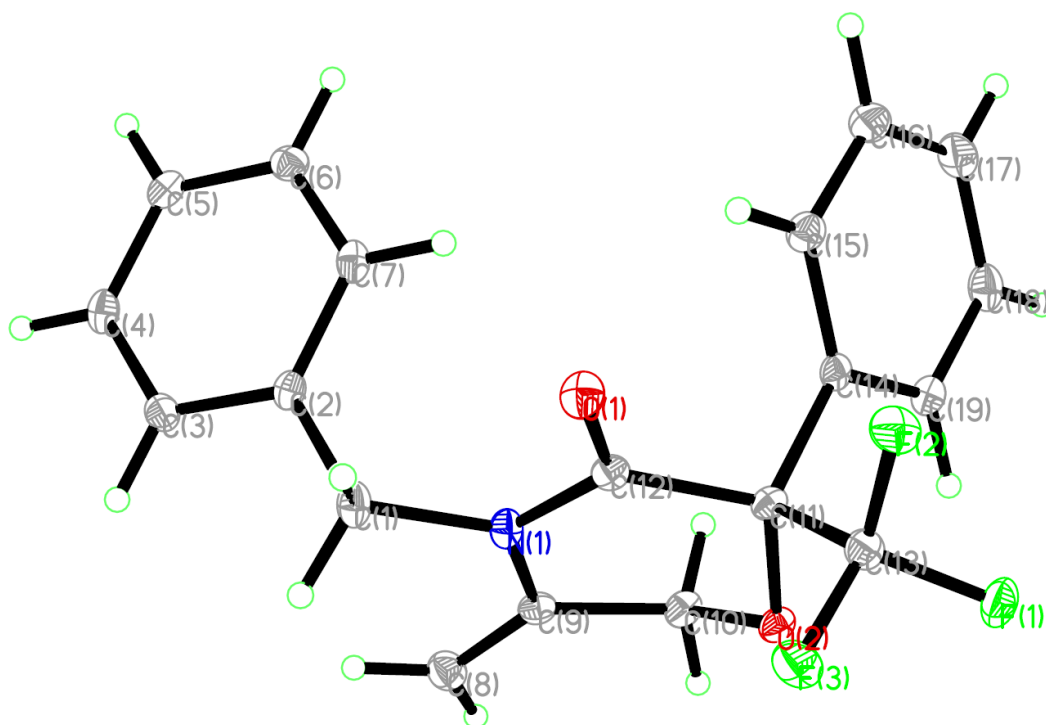


Table 1. Crystal data and structure refinement for 2a.

Identification code	shelx
Empirical formula	C <sub>19</sub> H <sub>16</sub> F <sub>3</sub> N O <sub>2</sub>
Formula weight	347.33
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.473(3) Å    alpha = 68.911(9) deg. b = 11.122(2) Å    beta = 89.618(10) deg. c = 14.777(4) Å    gamma = 83.233(9) deg.
Volume	1593.7(7) Å <sup>3</sup>
Z, Calculated density	4, 1.448 Mg/m <sup>3</sup>
Absorption coefficient	0.117 mm <sup>-1</sup>
F(000)	720
Crystal size	0.20 x 0.12 x 0.10 mm
Theta range for data collection	1.48 to 27.88 deg.
Limiting indices	-13 ≤ h ≤ 13, -12 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected / unique	16896 / 7492 [R(int) = 0.0381]
Completeness to theta = 27.88	98.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9884 and 0.9769
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	7492 / 0 / 451
Goodness-of-fit on F <sup>2</sup>	1.071
Final R indices [I > 2sigma(I)]	R1 = 0.0401, wR2 = 0.0837

R indices (all data) R1 = 0.0622, wR2 = 0.0890  
Largest diff. peak and hole 1.120 and -0.341 e.A<sup>-3</sup>

Table 2. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (A<sup>2</sup> x 10<sup>3</sup>) for 2a.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	394(1)	9067(1)	950(1)	29(1)
F(2)	2434(1)	8665(1)	1242(1)	28(1)
F(3)	1419(1)	7293(1)	903(1)	29(1)
F(4)	7068(1)	1039(1)	3858(1)	30(1)
F(5)	5014(1)	1437(1)	3890(1)	34(1)
F(6)	6225(1)	2754(1)	4109(1)	35(1)
O(1)	3197(1)	6261(1)	2676(1)	25(1)
O(2)	-185(1)	7132(1)	2448(1)	20(1)
O(3)	8204(1)	3100(1)	2571(1)	28(1)
O(4)	4792(1)	3553(1)	2380(1)	22(1)
N(1)	1614(1)	5088(1)	3458(1)	19(1)
N(2)	6858(1)	4870(1)	1634(1)	19(1)
C(1)	2551(2)	3904(1)	3812(1)	23(1)
C(2)	3004(1)	3533(1)	4858(1)	19(1)
C(3)	3089(2)	2247(1)	5485(1)	23(1)
C(4)	3603(2)	1867(2)	6428(1)	26(1)
C(5)	4039(2)	2780(2)	6746(1)	23(1)
C(6)	3955(2)	4067(2)	6129(1)	23(1)
C(7)	3438(2)	4440(1)	5193(1)	22(1)
C(8)	-183(2)	3896(2)	4152(1)	27(1)
C(9)	308(2)	4999(2)	3690(1)	20(1)
C(10)	-510(2)	6284(1)	3392(1)	21(1)
C(11)	1087(1)	7439(1)	2469(1)	17(1)
C(12)	2067(2)	6208(1)	2875(1)	19(1)
C(13)	1348(2)	8115(1)	1383(1)	22(1)
C(14)	1212(2)	8380(1)	3004(1)	18(1)
C(15)	2398(2)	8520(1)	3347(1)	24(1)
C(16)	2479(2)	9409(2)	3805(1)	30(1)
C(17)	1374(2)	10148(2)	3921(1)	31(1)
C(18)	197(2)	10027(2)	3574(1)	29(1)
C(19)	111(2)	9146(1)	3109(1)	22(1)
C(20)	7913(2)	5680(2)	1420(1)	24(1)

C(21)	8247(1)	6152(1)	357(1)	21(1)
C(22)	8500(2)	7421(2)	-111(1)	28(1)
C(23)	8855(2)	7852(2)	-1072(1)	34(1)
C(24)	8961(2)	7014(2)	-1576(1)	29(1)
C(25)	8710(2)	5753(2)	-1116(1)	26(1)
C(26)	8354(2)	5318(2)	-157(1)	24(1)
C(27)	5303(2)	6727(1)	781(1)	26(1)
C(28)	5601(2)	5460(1)	1267(1)	18(1)
C(29)	4624(2)	4538(1)	1431(1)	22(1)
C(30)	5999(2)	2779(1)	2498(1)	18(1)
C(31)	7124(2)	3596(1)	2241(1)	19(1)
C(32)	6088(2)	1996(2)	3598(1)	25(1)
C(33)	6022(2)	1842(1)	1939(1)	18(1)
C(34)	7161(2)	1398(1)	1601(1)	23(1)
C(35)	7146(2)	518(2)	1133(1)	28(1)
C(36)	6004(2)	78(2)	1004(1)	31(1)
C(37)	4867(2)	519(2)	1334(1)	29(1)
C(38)	4877(2)	1404(1)	1802(1)	24(1)

Table 3. Bond lengths [Å] and angles [deg] for 2a.

F(1)-C(13)	1.3417(17)
F(2)-C(13)	1.3341(17)
F(3)-C(13)	1.3396(15)
F(4)-C(32)	1.3363(18)
F(5)-C(32)	1.3420(18)
F(6)-C(32)	1.3374(16)
O(1)-C(12)	1.2214(18)
O(2)-C(11)	1.4169(17)
O(2)-C(10)	1.4405(16)
O(3)-C(31)	1.2198(18)
O(4)-C(30)	1.4170(17)
O(4)-C(29)	1.4318(17)
N(1)-C(12)	1.3710(18)
N(1)-C(9)	1.4135(19)
N(1)-C(1)	1.4758(18)
N(2)-C(31)	1.3731(18)
N(2)-C(28)	1.4168(19)
N(2)-C(20)	1.4690(18)
C(1)-C(2)	1.513(2)
C(1)-H(1A)	0.9900

C(1)-H(1B)	0.9900
C(2)-C(3)	1.389(2)
C(2)-C(7)	1.3929(19)
C(3)-C(4)	1.394(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.386(2)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.334(2)
C(8)-H(8A)	0.9500
C(8)-H(8B)	0.9500
C(9)-C(10)	1.494(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(14)	1.5385(19)
C(11)-C(12)	1.541(2)
C(11)-C(13)	1.5451(19)
C(14)-C(15)	1.390(2)
C(14)-C(19)	1.393(2)
C(15)-C(16)	1.395(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.385(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.378(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.394(2)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.519(2)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.387(2)
C(21)-C(26)	1.3888(19)
C(22)-C(23)	1.390(2)
C(22)-H(22)	0.9500
C(23)-C(24)	1.382(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.377(2)
C(24)-H(24)	0.9500

C(25)-C(26)	1.388(2)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(28)	1.330(2)
C(27)-H(27A)	0.9500
C(27)-H(27B)	0.9500
C(28)-C(29)	1.491(2)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-C(31)	1.535(2)
C(30)-C(32)	1.541(2)
C(30)-C(33)	1.5435(18)
C(33)-C(38)	1.389(2)
C(33)-C(34)	1.395(2)
C(34)-C(35)	1.3883(19)
C(34)-H(34)	0.9500
C(35)-C(36)	1.383(2)
C(35)-H(35)	0.9500
C(36)-C(37)	1.386(2)
C(36)-H(36)	0.9500
C(37)-C(38)	1.392(2)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(11)-O(2)-C(10)	110.71(10)
C(30)-O(4)-C(29)	111.30(11)
C(12)-N(1)-C(9)	123.84(13)
C(12)-N(1)-C(1)	116.93(13)
C(9)-N(1)-C(1)	119.14(13)
C(31)-N(2)-C(28)	123.12(13)
C(31)-N(2)-C(20)	118.04(13)
C(28)-N(2)-C(20)	118.67(12)
N(1)-C(1)-C(2)	113.71(11)
N(1)-C(1)-H(1A)	108.8
C(2)-C(1)-H(1A)	108.8
N(1)-C(1)-H(1B)	108.8
C(2)-C(1)-H(1B)	108.8
H(1A)-C(1)-H(1B)	107.7
C(3)-C(2)-C(7)	118.54(13)
C(3)-C(2)-C(1)	120.03(13)
C(7)-C(2)-C(1)	121.23(13)
C(2)-C(3)-C(4)	120.91(14)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5



C(5)-C(4)-C(3)	119.76(14)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	119.90(14)
C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	120.1
C(5)-C(6)-C(7)	120.08(14)
C(5)-C(6)-H(6)	120.0
C(7)-C(6)-H(6)	120.0
C(6)-C(7)-C(2)	120.80(14)
C(6)-C(7)-H(7)	119.6
C(2)-C(7)-H(7)	119.6
C(9)-C(8)-H(8A)	120.0
C(9)-C(8)-H(8B)	120.0
H(8A)-C(8)-H(8B)	120.0
C(8)-C(9)-N(1)	124.96(15)
C(8)-C(9)-C(10)	121.19(15)
N(1)-C(9)-C(10)	113.83(13)
O(2)-C(10)-C(9)	111.00(12)
O(2)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10A)	109.4
O(2)-C(10)-H(10B)	109.4
C(9)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
O(2)-C(11)-C(14)	112.71(12)
O(2)-C(11)-C(12)	111.68(12)
C(14)-C(11)-C(12)	111.71(12)
O(2)-C(11)-C(13)	103.16(11)
C(14)-C(11)-C(13)	109.44(11)
C(12)-C(11)-C(13)	107.65(11)
O(1)-C(12)-N(1)	122.80(14)
O(1)-C(12)-C(11)	119.76(14)
N(1)-C(12)-C(11)	117.44(13)
F(2)-C(13)-F(3)	107.45(12)
F(2)-C(13)-F(1)	106.53(12)
F(3)-C(13)-F(1)	107.04(12)
F(2)-C(13)-C(11)	112.97(12)
F(3)-C(13)-C(11)	112.19(12)
F(1)-C(13)-C(11)	110.31(12)
C(15)-C(14)-C(19)	119.56(14)
C(15)-C(14)-C(11)	121.69(13)
C(19)-C(14)-C(11)	118.69(14)
C(14)-C(15)-C(16)	120.10(15)

C(14)-C(15)-H(15)	119.9
C(16)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	119.79(16)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(18)-C(17)-C(16)	120.51(15)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	119.96(16)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(14)-C(19)-C(18)	120.06(16)
C(14)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
N(2)-C(20)-C(21)	113.23(11)
N(2)-C(20)-H(20A)	108.9
C(21)-C(20)-H(20A)	108.9
N(2)-C(20)-H(20B)	108.9
C(21)-C(20)-H(20B)	108.9
H(20A)-C(20)-H(20B)	107.7
C(22)-C(21)-C(26)	118.60(14)
C(22)-C(21)-C(20)	120.22(13)
C(26)-C(21)-C(20)	121.13(13)
C(21)-C(22)-C(23)	120.87(14)
C(21)-C(22)-H(22)	119.6
C(23)-C(22)-H(22)	119.6
C(24)-C(23)-C(22)	120.05(15)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(25)-C(24)-C(23)	119.40(15)
C(25)-C(24)-H(24)	120.3
C(23)-C(24)-H(24)	120.3
C(24)-C(25)-C(26)	120.74(14)
C(24)-C(25)-H(25)	119.6
C(26)-C(25)-H(25)	119.6
C(25)-C(26)-C(21)	120.34(15)
C(25)-C(26)-H(26)	119.8
C(21)-C(26)-H(26)	119.8
C(28)-C(27)-H(27A)	120.0
C(28)-C(27)-H(27B)	120.0
H(27A)-C(27)-H(27B)	120.0
C(27)-C(28)-N(2)	123.72(15)
C(27)-C(28)-C(29)	121.59(15)

N(2)-C(28)-C(29)	114.64(12)
O(4)-C(29)-C(28)	111.24(12)
O(4)-C(29)-H(29A)	109.4
C(28)-C(29)-H(29A)	109.4
O(4)-C(29)-H(29B)	109.4
C(28)-C(29)-H(29B)	109.4
H(29A)-C(29)-H(29B)	108.0
O(4)-C(30)-C(31)	112.43(12)
O(4)-C(30)-C(32)	102.35(11)
C(31)-C(30)-C(32)	108.45(12)
O(4)-C(30)-C(33)	111.76(12)
C(31)-C(30)-C(33)	111.80(12)
C(32)-C(30)-C(33)	109.56(11)
O(3)-C(31)-N(2)	122.86(14)
O(3)-C(31)-C(30)	119.64(13)
N(2)-C(31)-C(30)	117.50(13)
F(4)-C(32)-F(6)	107.69(13)
F(4)-C(32)-F(5)	106.62(12)
F(6)-C(32)-F(5)	107.03(12)
F(4)-C(32)-C(30)	112.80(12)
F(6)-C(32)-C(30)	111.60(12)
F(5)-C(32)-C(30)	110.80(13)
C(38)-C(33)-C(34)	119.72(13)
C(38)-C(33)-C(30)	118.39(13)
C(34)-C(33)-C(30)	121.86(14)
C(35)-C(34)-C(33)	119.95(15)
C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0
C(36)-C(35)-C(34)	120.08(16)
C(36)-C(35)-H(35)	120.0
C(34)-C(35)-H(35)	120.0
C(35)-C(36)-C(37)	120.35(15)
C(35)-C(36)-H(36)	119.8
C(37)-C(36)-H(36)	119.8
C(36)-C(37)-C(38)	119.80(16)
C(36)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
C(33)-C(38)-C(37)	120.10(15)
C(33)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 2a.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
F(1)	34(1)	24(1)	21(1)	0(1)	-4(1)	1(1)
F(2)	30(1)	31(1)	23(1)	-7(1)	8(1)	-13(1)
F(3)	44(1)	28(1)	20(1)	-12(1)	6(1)	-9(1)
F(4)	39(1)	22(1)	23(1)	-4(1)	-4(1)	5(1)
F(5)	40(1)	32(1)	26(1)	-4(1)	13(1)	-8(1)
F(6)	59(1)	27(1)	21(1)	-12(1)	0(1)	-1(1)
O(1)	18(1)	28(1)	29(1)	-9(1)	6(1)	-2(1)
O(2)	18(1)	22(1)	16(1)	-3(1)	0(1)	-5(1)
O(3)	22(1)	26(1)	35(1)	-8(1)	-7(1)	0(1)
O(4)	20(1)	21(1)	21(1)	-4(1)	5(1)	1(1)
N(1)	22(1)	18(1)	17(1)	-5(1)	2(1)	1(1)
N(2)	18(1)	17(1)	19(1)	-5(1)	0(1)	-3(1)
C(1)	28(1)	20(1)	19(1)	-6(1)	3(1)	3(1)
C(2)	17(1)	20(1)	18(1)	-5(1)	3(1)	1(1)
C(3)	26(1)	19(1)	24(1)	-9(1)	1(1)	-2(1)
C(4)	29(1)	20(1)	23(1)	-2(1)	-1(1)	3(1)
C(5)	19(1)	27(1)	21(1)	-6(1)	-1(1)	0(1)
C(6)	18(1)	26(1)	27(1)	-11(1)	2(1)	-4(1)
C(7)	19(1)	18(1)	23(1)	-3(1)	6(1)	-1(1)
C(8)	32(1)	25(1)	26(1)	-9(1)	2(1)	-6(1)
C(9)	21(1)	24(1)	15(1)	-8(1)	1(1)	-4(1)
C(10)	19(1)	25(1)	17(1)	-3(1)	3(1)	-5(1)
C(11)	15(1)	21(1)	16(1)	-6(1)	1(1)	-3(1)
C(12)	21(1)	22(1)	14(1)	-8(1)	1(1)	-2(1)
C(13)	24(1)	21(1)	19(1)	-7(1)	2(1)	-4(1)
C(14)	22(1)	17(1)	12(1)	-2(1)	1(1)	-2(1)
C(15)	25(1)	25(1)	20(1)	-8(1)	-1(1)	-1(1)
C(16)	36(1)	29(1)	23(1)	-7(1)	-6(1)	-7(1)
C(17)	50(1)	25(1)	22(1)	-12(1)	-1(1)	-4(1)
C(18)	36(1)	21(1)	27(1)	-8(1)	3(1)	3(1)
C(19)	22(1)	22(1)	20(1)	-5(1)	1(1)	0(1)
C(20)	25(1)	23(1)	26(1)	-10(1)	-2(1)	-8(1)
C(21)	15(1)	23(1)	23(1)	-6(1)	-1(1)	-4(1)
C(22)	29(1)	23(1)	33(1)	-11(1)	4(1)	-8(1)
C(23)	36(1)	23(1)	38(1)	-3(1)	8(1)	-9(1)
C(24)	23(1)	35(1)	23(1)	-4(1)	2(1)	-4(1)
C(25)	24(1)	30(1)	26(1)	-12(1)	1(1)	-5(1)

C(26)	23(1)	21(1)	25(1)	-6(1)	-2(1)	-5(1)
C(27)	27(1)	23(1)	25(1)	-6(1)	2(1)	0(1)
C(28)	20(1)	21(1)	15(1)	-8(1)	2(1)	0(1)
C(29)	20(1)	23(1)	19(1)	-5(1)	-1(1)	2(1)
C(30)	18(1)	18(1)	17(1)	-5(1)	1(1)	1(1)
C(31)	20(1)	21(1)	17(1)	-9(1)	-1(1)	-1(1)
C(32)	32(1)	21(1)	22(1)	-9(1)	3(1)	-2(1)
C(33)	23(1)	15(1)	13(1)	-2(1)	0(1)	-2(1)
C(34)	24(1)	23(1)	19(1)	-7(1)	2(1)	-1(1)
C(35)	39(1)	24(1)	19(1)	-7(1)	1(1)	5(1)
C(36)	56(1)	19(1)	19(1)	-7(1)	-6(1)	0(1)
C(37)	39(1)	22(1)	24(1)	-3(1)	-9(1)	-9(1)
C(38)	26(1)	22(1)	20(1)	-3(1)	-1(1)	-3(1)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 2a.

	x	y	z	U(eq)
H(1A)	3307	4038	3397	28
H(1B)	2154	3174	3744	28
H(3)	2792	1618	5268	27
H(4)	3654	985	6850	31
H(5)	4396	2524	7387	28
H(6)	4251	4694	6348	28
H(7)	3378	5325	4776	26
H(8A)	357	3090	4351	33
H(8B)	-1074	3916	4281	33
H(10A)	-1427	6152	3379	26
H(10B)	-386	6693	3875	26
H(15)	3153	8008	3270	29
H(16)	3289	9507	4037	36
H(17)	1428	10743	4243	38
H(18)	-555	10543	3651	35
H(19)	-699	9069	2864	27
H(20A)	8687	5173	1818	29
H(20B)	7669	6442	1609	29
H(22)	8429	8003	230	33
H(23)	9026	8724	-1383	40
H(24)	9204	7305	-2233	35
H(25)	8782	5174	-1460	31
H(26)	8182	4446	150	28

H(27A)	5950	7290	663	31
H(27B)	4442	7068	552	31
H(29A)	3751	5022	1356	26
H(29B)	4702	4126	938	26
H(34)	7946	1698	1690	27
H(35)	7920	217	901	34
H(36)	5998	-530	688	38
H(37)	4084	219	1241	35
H(38)	4099	1708	2028	29

Table 6. Torsion angles [deg] for 2a.

C(12)-N(1)-C(1)-C(2)	102.79(15)
C(9)-N(1)-C(1)-C(2)	-80.54(17)
N(1)-C(1)-C(2)-C(3)	135.62(15)
N(1)-C(1)-C(2)-C(7)	-49.4(2)
C(7)-C(2)-C(3)-C(4)	-0.4(2)
C(1)-C(2)-C(3)-C(4)	174.68(14)
C(2)-C(3)-C(4)-C(5)	-0.1(2)
C(3)-C(4)-C(5)-C(6)	0.4(2)
C(4)-C(5)-C(6)-C(7)	-0.2(2)
C(5)-C(6)-C(7)-C(2)	-0.4(2)
C(3)-C(2)-C(7)-C(6)	0.7(2)
C(1)-C(2)-C(7)-C(6)	-174.37(14)
C(12)-N(1)-C(9)-C(8)	171.14(13)
C(1)-N(1)-C(9)-C(8)	-5.3(2)
C(12)-N(1)-C(9)-C(10)	-10.54(19)
C(1)-N(1)-C(9)-C(10)	173.05(11)
C(11)-O(2)-C(10)-C(9)	-64.80(15)
C(8)-C(9)-C(10)-O(2)	-140.35(13)
N(1)-C(9)-C(10)-O(2)	41.25(17)
C(10)-O(2)-C(11)-C(14)	-72.52(14)
C(10)-O(2)-C(11)-C(12)	54.21(14)
C(10)-O(2)-C(11)-C(13)	169.55(10)
C(9)-N(1)-C(12)-O(1)	-179.26(13)
C(1)-N(1)-C(12)-O(1)	-2.8(2)
C(9)-N(1)-C(12)-C(11)	1.21(19)
C(1)-N(1)-C(12)-C(11)	177.71(11)
O(2)-C(11)-C(12)-O(1)	157.60(12)
C(14)-C(11)-C(12)-O(1)	-75.13(16)
C(13)-C(11)-C(12)-O(1)	45.04(18)

O(2)-C(11)-C(12)-N(1)	-22.86(16)
C(14)-C(11)-C(12)-N(1)	104.41(15)
C(13)-C(11)-C(12)-N(1)	-135.42(12)
O(2)-C(11)-C(13)-F(2)	170.40(11)
C(14)-C(11)-C(13)-F(2)	50.20(16)
C(12)-C(11)-C(13)-F(2)	-71.40(15)
O(2)-C(11)-C(13)-F(3)	-67.95(14)
C(14)-C(11)-C(13)-F(3)	171.85(13)
C(12)-C(11)-C(13)-F(3)	50.25(16)
O(2)-C(11)-C(13)-F(1)	51.30(14)
C(14)-C(11)-C(13)-F(1)	-68.90(15)
C(12)-C(11)-C(13)-F(1)	169.50(12)
O(2)-C(11)-C(14)-C(15)	161.42(13)
C(12)-C(11)-C(14)-C(15)	34.71(19)
C(13)-C(11)-C(14)-C(15)	-84.41(16)
O(2)-C(11)-C(14)-C(19)	-21.21(18)
C(12)-C(11)-C(14)-C(19)	-147.92(13)
C(13)-C(11)-C(14)-C(19)	92.96(16)
C(19)-C(14)-C(15)-C(16)	0.9(2)
C(11)-C(14)-C(15)-C(16)	178.20(13)
C(14)-C(15)-C(16)-C(17)	0.3(2)
C(15)-C(16)-C(17)-C(18)	-1.0(2)
C(16)-C(17)-C(18)-C(19)	0.6(2)
C(15)-C(14)-C(19)-C(18)	-1.3(2)
C(11)-C(14)-C(19)-C(18)	-178.74(13)
C(17)-C(18)-C(19)-C(14)	0.6(2)
C(31)-N(2)-C(20)-C(21)	115.90(14)
C(28)-N(2)-C(20)-C(21)	-68.75(16)
N(2)-C(20)-C(21)-C(22)	137.85(15)
N(2)-C(20)-C(21)-C(26)	-44.6(2)
C(26)-C(21)-C(22)-C(23)	-0.2(2)
C(20)-C(21)-C(22)-C(23)	177.45(15)
C(21)-C(22)-C(23)-C(24)	0.0(3)
C(22)-C(23)-C(24)-C(25)	0.0(3)
C(23)-C(24)-C(25)-C(26)	0.0(2)
C(24)-C(25)-C(26)-C(21)	-0.1(2)
C(22)-C(21)-C(26)-C(25)	0.2(2)
C(20)-C(21)-C(26)-C(25)	-177.39(14)
C(31)-N(2)-C(28)-C(27)	171.23(13)
C(20)-N(2)-C(28)-C(27)	-3.87(19)
C(31)-N(2)-C(28)-C(29)	-11.14(18)
C(20)-N(2)-C(28)-C(29)	173.76(11)
C(30)-O(4)-C(29)-C(28)	-62.97(14)

C(27)-C(28)-C(29)-O(4)	-141.56(13)
N(2)-C(28)-C(29)-O(4)	40.75(16)
C(29)-O(4)-C(30)-C(31)	52.93(14)
C(29)-O(4)-C(30)-C(32)	169.09(11)
C(29)-O(4)-C(30)-C(33)	-73.76(14)
C(28)-N(2)-C(31)-O(3)	-178.39(13)
C(20)-N(2)-C(31)-O(3)	-3.3(2)
C(28)-N(2)-C(31)-C(30)	1.94(19)
C(20)-N(2)-C(31)-C(30)	177.06(11)
O(4)-C(30)-C(31)-O(3)	157.79(12)
C(32)-C(30)-C(31)-O(3)	45.35(17)
C(33)-C(30)-C(31)-O(3)	-75.56(16)
O(4)-C(30)-C(31)-N(2)	-22.53(17)
C(32)-C(30)-C(31)-N(2)	-134.97(13)
C(33)-C(30)-C(31)-N(2)	104.12(14)
O(4)-C(30)-C(32)-F(4)	169.93(12)
C(31)-C(30)-C(32)-F(4)	-71.07(15)
C(33)-C(30)-C(32)-F(4)	51.21(17)
O(4)-C(30)-C(32)-F(6)	-68.68(15)
C(31)-C(30)-C(32)-F(6)	50.32(17)
C(33)-C(30)-C(32)-F(6)	172.60(13)
O(4)-C(30)-C(32)-F(5)	50.48(14)
C(31)-C(30)-C(32)-F(5)	169.48(11)
C(33)-C(30)-C(32)-F(5)	-68.23(16)
O(4)-C(30)-C(33)-C(38)	-29.43(17)
C(31)-C(30)-C(33)-C(38)	-156.45(13)
C(32)-C(30)-C(33)-C(38)	83.29(16)
O(4)-C(30)-C(33)-C(34)	152.64(13)
C(31)-C(30)-C(33)-C(34)	25.61(19)
C(32)-C(30)-C(33)-C(34)	-94.65(16)
C(38)-C(33)-C(34)-C(35)	-0.3(2)
C(30)-C(33)-C(34)-C(35)	177.62(13)
C(33)-C(34)-C(35)-C(36)	-0.2(2)
C(34)-C(35)-C(36)-C(37)	0.5(2)
C(35)-C(36)-C(37)-C(38)	-0.4(2)
C(34)-C(33)-C(38)-C(37)	0.4(2)
C(30)-C(33)-C(38)-C(37)	-177.57(13)
C(36)-C(37)-C(38)-C(33)	-0.1(2)

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Symmetry transformations used to generate equivalent atoms: